

CHANGING THE LOGIC OF SCIENCE

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A Bayesian Interpretation of Quantum Mechanics

JOHN HEMP

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Preface

This monograph is devoted to an interpretation of non-relativistic quantum mechanics.

The ideas in it came by degrees after I discovered the work of E. T. Jaynes, first various conference papers of his and then his book ‘Probability Theory –The Logic of Science’ published in 2003 shortly after his death. In my opinion Jaynes’ contribution to probability theory has been immense. He demonstrated the power of the rational Bayesian interpretation which makes probability an extension of logic allowing for degrees of belief given limited knowledge. So probability it seems is rational degree of belief given limited knowledge - not (as most physicists seem to think) relative frequency (in repeated trials) under specified physical conditions.*

Another great source of inspiration was the work of R. P. Feynman regarding the interpretation of quantum mechanics: especially in the presentation of the subject in Volume III of ‘The Feynman Lectures on Physics’ and in the book written with A. R. Hibbs entitled ‘Quantum Mechanics and Path Integrals’. As is well known, Feynman worked with ‘probability amplitudes’ and noted that these were related to each other in a way similar to the way ordinary probabilities are related. But he stopped short of interpreting probability amplitudes directly as probabilities because they were complex-valued rather than real and positive, and because he adopted a frequency interpretation of probability rather than a Bayesian one.

But if probabilities are not relative frequencies but degrees of belief is it not possible that the probability of an event might be represented by a complex number?† Also, viewed from a rational Bayesian perspective, might not the laws of probability have to change on account of the *uncertainty principle* – i.e. on account of the fact that acquisition of knowledge of a quantum process generally affects it physically and we are unable to hold knowledge of incompatible physical properties simultaneously? It was roughly with these thoughts that I started (in 2002) on the road that has led to this monograph.

This monograph presents my best attempt so far to turn ‘probability amplitudes’ into actual (complex valued) probabilities obeying a new complex-valued probability calculus that takes account (in a general way) of the uncontrollable physical interaction accompanying acquisition of knowledge and is consistent with the existing quantum mechanical formalism. The result is a new logic of science, and using it we are free to postulate new physical laws that are purely objective. It does not matter how strange these laws may have to be so long as they are consistent and conceivably true and of course so long as they lead (through the new probability calculus) to the usual predictions of quantum mechanics. With a certain choice of such new physical laws, application of the new probability calculus including its rules for forming prior probability distributions (extensions of the principle of indifference, the method of transformation groups, etc.),

* Of course probability is *sometimes* numerically *equal* to *expected* relative frequency under specified physical conditions.

† with the modulus squared of this number, rather than the number itself, sometimes equal to the expected relative frequency of the event in repeated trials

leads to the usual forms of the Schrödinger equation and to the usual relations between wave functions in different representations and so on.*

It is possible the interpretation contains hidden ambiguities or inconsistencies. Many have arisen during its construction but a natural way of avoiding them has each time been found with the result that the theory is better than before. This process of constant adjustment may have reached an end now. The interpretation may now be free from ambiguity and contradiction. But even if it is not yet right or complete it may provide ideas for the formulation of the correct interpretation.

Only non-relativistic quantum theory is considered.† It is surely necessary first to fully interpret the non-relativistic theory before going on to consider the relativistic theory. Non-relativistic quantum theory is complete in itself and easier to interpret than relativistic quantum theory. The lessons to be learnt are hard enough without relativistic complications. But of course the real gains of the approach may come in its application to the relativistic case when perhaps much bigger changes in ideas will be necessary.

J.H. ‡

* The present theory may therefore at least come close to achieving the objective advocated by Jaynes when he says: “We believe that to achieve a rational picture of the world it is necessary to set up another clear division of labour within theoretical physics; it is the job of the laws of physics to describe physical causation at the level of ontology, and the job of probability theory to describe human inferences at the level of epistemology. The Copenhagen theory scrambles these very different functions into a nasty omelette in which the distinction between reality and our knowledge of reality is lost.” See ‘Clearing up Mysteries – The Original Goal’ by E. T. Jaynes in ‘Maximum Entropy and Bayesian Methods’ Ed. J. Skilling, Cambridge England, 1988, Kluwer Academic Publishers.

† Certain parts of the non-relativistic theory are not covered in this monograph (e.g. non-relativistic second quantisation). But enough is covered here I think to make the case for the general interpretation.

‡ Before retirement in 2002, the author was a senior lecturer in the School of Engineering, Cranfield University, Bedfordshire, UK. He is presently a Member of Common Room at Wolfson College, Oxford, UK.

Introduction

1. The meaning of probability

For the purpose of interpreting quantum mechanics and for changing the laws of probability to take account of quantum mechanical uncertainty we adopt the rational Bayesian interpretation of probability as advocated, for example by Jaynes [2] and many before him such as Laplace, Maxwell, Keynes and Jeffreys so when we speak of ‘probability’ we will always mean probability in a rational Bayesian sense. We thus take probability theory to be an extension of logic, to take account of and to quantify uncertainty in our beliefs given our knowledge. We agree with Jaynes (and others) that this is the true nature of probability and that probability is not a measure of frequency or propensity.

The interpretation of probability adopted is thus the more subjective of the two interpretations of what is sometimes called the ‘logical theory of probability’*. We will thus talk of probability as quantifying our ‘rational state of belief given our (actual or supposed) knowledge’. This interpretation is objective in so much as the probabilities (correctly) calculated by different people (given the same information) are always the same. In adopting this Bayesian interpretation of probability rather than the usual frequency interpretation we free ourselves from the need for probabilities to be represented by real positive numbers. We suppose instead each probability is represented by a complex number. The squared modulus of this complex number will be a measure of our degree of belief and its argument will be called our ‘phase of belief’. Two real numbers will therefore be required to fully quantify our rational state of belief in a proposition given our (actual or supposed) knowledge.

It may be as well to point out here that ‘our (actual or supposed) knowledge’ will be expressed by propositions of three kinds; propositions claiming relevant general knowledge (the laws of quantum mechanics and of probability theory), propositions claiming certain unchanging properties of the physical processes under study, and propositions claiming specific dynamical properties of the physical processes (in the macro-world or in the micro-world)†. Only knowledge expressed by propositions of the latter kind is subject to the uncertainty principle.

*According to one interpretation of the logical theory of probability (see pp29-33 of [1]) probability is described as being the ‘degree of corroboration (or of partial entailment) of one proposition by another’. According to the other it is ‘the degree of belief we should rationally hold in one proposition given we *know* another to be true’. In classical probability used with classical physics there is not much difference between these interpretations because we can always *suppose we know* of the truth of a (conditional) proposition on which a probability depends, and then ‘degree of belief’ and ‘degree of partial entailment’ can surely be assumed equal. The acquisition of knowledge is not problematic in classical physics. But in quantum physics it *is* problematic because of the uncertainty principle. It is for this reason that a definite choice has to be made regarding the two interpretations of the logical theory of probability. As we wish to calculate probabilities on the basis of knowledge acquired and to take into account the possible physical effects of acquiring that knowledge we have to choose the second interpretation.

† In the macro-world these include propositions about the readings of measuring apparatus. In the micro-world these are propositions about the dynamical properties of atomic or molecular systems whose truth or

We will not be trying to calculate probabilities conditional on propositions claiming unverified dynamical properties of the micro-world (such as through which slit a particle is supposed to have passed in a double slit experiment). These propositions do not constitute (actual or supposed) *knowledge*. We *will* be trying to calculate probabilities conditional on propositions claiming we *know* certain dynamical properties of the micro-world (such as which slit a particle passed through).*

2. The present interpretation of quantum mechanics and its relation to the normal interpretation

2.1 Wave functions and properties

In the usual interpretation of quantum mechanics it is denied that systems *possess* dynamical properties. For example a single quantum mechanical particle is not said to *possess* properties like position, momentum, ...etc. Instead it is claimed only that a particle can interact with macroscopic measuring apparatus to give macroscopic outcomes that can be referred to as '*measurements* of position, momentum, ... etc'. But research into the foundations of quantum mechanics has shown that ordinary possession of properties *can* be consistent with the quantum formalism at least if restriction is made to possession of properties that are represented by *complete sets* of commuting observables in Hilbert space. This way the Kochen-Specker paradox can be avoided (see page 134 of [4]). In connection with a single system we too will avoid claiming that *every* observable represents a property and we too will assume that complete sets of commuting observables represent properties possessed by the system. (Of course, any function of a complete set of commuting observables also represents a possessed property going with that complete set. For example, one component (say the x component) of momentum of a particle is a property going with the (vector) momentum, the three Cartesian components of which together form a complete set in regard to the motion of a single particle system. And the kinetic energy of a free particle, defined as the sum of the squares of the three Cartesian components of momentum divided by twice the particle mass, is a property going with the three Cartesian components of momentum.)

When the tensor product of Hilbert spaces is taken to represent the states of two or more systems (in interaction or not), the complete sets of commuting observables in the component Hilbert spaces cease to be complete sets in the product space but this particular case does not, it seems, lead to a Kochen-Specker type Paradox (see page 140 of [4]), i.e. complete sets in the component Hilbert spaces can still represent properties possessed by the whole system and we too assume this is so.

falsity may sometimes be inferred (with the help of our general knowledge) from the (directly observable) readings of our measuring apparatus.

* If one is not a convinced and practiced Bayesian already it is quite a struggle to convert oneself to the Bayesian philosophy. One must constantly remember to make all probabilities (whether classical or complex-valued) conditional on the (actual or supposed) knowledge of the reasoner and not on the (actual or supposed) physical conditions present. It is not physical conditions that determine probabilities but knowledge.

In the quantum mechanical formalism, the projections (at any one time) of the (normalised) state vector in Hilbert space onto the eigenvectors of a complete set of commuting observables gives a set of complex numbers called a wave function. In this monograph the state vector represents our *knowledge* regarding the motion of the system in question. And we take each wave function to be the (complex-valued) probability distribution we should adopt over the possible values of the complete set of observables in question given that knowledge.

In the normal interpretation of quantum mechanics a wave function is taken to represent the momentary physical state of a system. This leads to the well known problem of wave function collapse - a physical process operating outside the dynamical laws of quantum mechanics. But it has been noted before (see for example [3]) that by supposing (as we do in this monograph) that a wave function is an expression only of our *knowledge* of the physical state, this problem is avoided. ‘Collapse of the wave function’ is then just a mental process resulting from the acquisition of new knowledge.

2.2 The uncertainty principle

In the usual interpretation of quantum mechanics the uncertainty principle expresses the general law that simultaneous measurement of incompatible properties (like position and momentum) is problematic because measurement of one might unpredictably alter the value of the other. This claim is backed up by physical arguments (as for example in [5] and [8]) based on assumed possession of the properties by the system. But the argument is usually taken further, i.e. the further claim is made that therefore properties (like position and momentum) are generally speaking *not actually possessed* by a system. In this monograph this further claim of the non-possession of key dynamical properties is regarded as a mind projection fallacy and is not made.* But the difficulty in principle of us acquiring simultaneous *knowledge* of incompatible properties (like the exact position and exact momentum of a particle in the present or at a time in the future) *is* granted and plays a fundamental role.

2.3 Pure states

In place of the possibility (in principle) of knowing all about a classical process we suppose the possibility (in principle) of preparing a quantum process in a ‘pure state’. In the present interpretation ‘pure state’ does not refer to a physical state of the process but rather to a pure state *of our knowledge* regarding the process. Whenever the term ‘pure state’ is employed in this monograph ‘pure state of knowledge’ will be meant. As soon as a process is prepared in a ‘pure state’ (for example by measurement of one dynamical property of the system at a certain time) we have a pure state of knowledge *Y* of the process as it freely evolves thereafter and, with regard to future properties of the process,

* Like Feynman and Hibbs (see section 1.3 of [16]), rather than blurring the possession of dynamical properties we seek instead to alter the laws of probability.

all previous knowledge about the process becomes redundant. We are then, in a sense, on the boundary of possible knowledge of the process. The acquisition of any *further* knowledge of the process is problematic because it carries with it the possibility of causing unpredictable changes in the process whose likely magnitude cannot be made arbitrarily small even in principle. But new information A may be obtained through ‘harmless conditioning’ (a filtration or null measurement). After harmless conditioning we gain more precise knowledge of *some* dynamical property of the process without affecting that property, but lose information about another, and, with regard to the future, some or all previous information becomes redundant but a new pure state is established associated with knowledge denoted by AY (i.e. by the conjunction of the propositions A and Y) or just by A if *all* previous information becomes redundant. In particular, a null measurement of particle position* at a specified time can succeed in instantaneously sharpening our knowledge of the particle’s position at that time producing a new pure state ‘harmlessly’ with regard to position, i.e. without affecting particle position *at the time in question*; but such a measurement might affect the particle’s *momentum* at the time in question and it might affect its position at *later* times, and as a result it generally renders less precise our knowledge regarding the particle’s momentum at the time in question and our knowledge regarding its position at a later time.

2.4 The calculation of probabilities

In classical (Bayesian) probability used with classical physics it is often possible by logical reasoning to deduce degrees of belief we should rationally hold in various propositions given our knowledge. This can be done using for example the principle of indifference or the principle of maximum entropy or the method of transformation groups. Jaynes [2] has carefully formulated the various principles and methods currently available for doing this. But the probabilities of some propositions given our knowledge are simply non-existent.† And although it may be true that research into the general problem of deducing rational (prior) probabilities from relevant knowledge is not yet over, it also seems likely that the probabilities of certain propositions given certain knowledge (while stated to be formally existent) cannot *in principle* be calculated; the knowledge may be insufficient or of the wrong kind.‡ There remain of course plenty of propositions whose probabilities *can* be deduced or calculated; enough to ensure the great utility of classical Bayesian probability and its superiority over other interpretations of probability.

* i.e. failure to find the particle in a certain region of space

† For example it is sometimes impossible to define a measure over *all* the subsets of a set Ω so, treating Ω as a sample space and a subset as an ‘event’, not all propositions claiming events can (consistently) have probabilities.

‡ For example, it would seem that the classical (prior) probability distribution $f(x)$ where x is a (continuous) real variable is indeterminate given that x lies between 0 and 1 and there is no natural measure over the interval $0 < x < 1$. A function $f(x)$ is calculable for each postulated natural measure, but if we know there is *no* natural measure $f(x)$ becomes *indeterminate*.

In the new (complex-valued) probability theory (including in its application to quantum mechanical systems), it will be possible to apply certain logical principles for calculating probabilities or establishing the form of prior distributions, but it will not be possible to deduce the (complex-valued) probabilities we should hold in *any* propositions given our knowledge. Some probabilities may be simply non-existent, like the probabilities in a *joint* probability distribution over the position and momentum of a particle under any pure knowledge of the particle's orbital motion.*

If our knowledge of a quantum mechanical system is pure it will be possible to determine the moduli and at least the *relative* phases of the (complex-valued) probabilities in certain important probability distributions. But under pure knowledge it can be that the phases of some probabilities whose moduli are calculable are indeterminate. This is generally the case for the probabilities of disjunctions of mutually exclusive propositions whose complex-valued probabilities may themselves be fully determinate.† And the *absolute* phases of the probabilities in the above mentioned important probability distributions are often incalculable (i.e. indeterminate) under pure knowledge, and their relative phases may be incalculable if our knowledge falls short of being pure. Those relative phases are then indeterminate, but it may well be possible to calculate the moduli of the probabilities given our knowledge.‡

For the purpose of calculating (complex-valued) probabilities under pure states of knowledge we place particular propositions about the physical world into certain categories ('complete sample spaces' of propositions and 'basic sets' of propositions within them) and lay down certain general laws of probability (sum rule, product rule, and laws of extreme values of probability) and certain general laws of logical implication (since implication now carries a phase). We also formulate certain rules for deducing prior probability distributions (extensions of the classical principles of indifference, transformation groups etc.). In some of these rules we allow, in a general way, for the possibility (on account of the uncertainty principle) that acquisition of knowledge may (unavoidably) change the truth values of propositions claiming physical properties. The uncertainty principle is thus built into the theory of probability itself. This reflects the

* Such probabilities, if they existed, could never be tested by determining the relative frequencies of measurement results because the uncertainty principle renders the necessary measurements impossible. And this is in keeping with the probabilities in question being non-existent.

† See the sum rule (section 2.3 of Chapter I).

‡ Quantum mechanics with indeterminate phases can be compared with the statics of statically-indeterminate pin-jointed frameworks. It may be that the phases of some probabilities in a quantum mechanical application (or the tensions or compressions in some of the members of a pin-jointed framework) cannot be determined theoretically. But indeterminacy of some parameters of a theory need not render the theory useless. For we may (without leading to contradiction) employ unevaluated parameters (i.e. algebraic symbols) to represent the indeterminate phases in the complex-valued probability application (or the indeterminate tensions or compressions in the pin-jointed framework). Then, using the laws of probability (or the laws of statics) other parameters in the quantum mechanical application (or in the theory of the pin-jointed framework) may be perfectly well and usefully calculated. There is then always the possibility of assigning, to within a certain freedom of choice, representative values to the indeterminate parameters such that all theoretically required relations between parameters are satisfied. Of course we cannot then claim our chosen parameter values are *correct*, they represent only a 'possibility'.

way the world is and our place in it. In order to make sense of the world this is how probability, as an extension of logic, must be formulated.*

The new theory of probability demonstratively reduces to the classical theory of probability under conditions in which we are prepared to work experimentally at an accuracy low enough to ensure the uncertainty principle does not have to play a significant part in our reasoning.

2.5 The laws of quantum mechanics in the present interpretation

The laws of quantum mechanics proposed in this work are of two sorts. There are laws concerning (i) the logical character of propositions about the physical world, and (ii) properties of the motion of quantum mechanical systems.

Laws of the second sort are natural laws of the kind claimed in classical physics. They establish certain definite relations between dynamical variables. Or they lay down general principles like the homogeneity and isotropy of space, the possibility of time reversal etc. But they do not amount to a system of deterministic laws like we have in classical mechanics. They are not as ‘complete’ as that and this seems naturally to reflect our inability (on account of the uncertainty principle) to confirm any proposed deterministic theory by measurement of all dynamical variables. But although our natural laws will not be ‘complete’ we must allow at least partial specification of *phases of implication* in these laws (see section 2.2.1 of Chapter I).

Laws of the first sort are needed to identify which propositions (about the physical process under study) fall into the various logical categories laid down in our theory of probability (see section 3.1 of Chapter I for example).

2.6 Derivation of the usual equations of quantum mechanics

Under the new (complex-valued) probability theory there is no uncertainty in the physical world itself. Everything there (every physical property) is supposed to be definite. But our *knowledge* of what is there can never be complete.

In the modelling of a quantum mechanical process we are free to propose laws of the two sorts described in section 2.5, i.e. to put certain propositions about the process into the established logical categories and to lay down physical laws making definite claims about properties of the process. But this cannot of course be done in just any way. It must be

* The inevitability of the historical variation of logic (or the laws of thought) was noted by Frederick Engels: ‘In every epoch ... theoretical thought is a historical product, which at different times assumes very different forms ... And this is of importance also for the practical application of thought in empirical fields. Because in the first place the theory of the laws of thought is by no means an “eternal truth” established once and for all, as philistine reasoning imagines to be the case with the word ‘logic’. Formal logic ... has [after all] been the arena of violent controversy from the time of Aristotle ...’ (p 44 of [17]).

done in a way that (on the basis of the complex-valued probability theory) agrees with the usual mathematical formalism of quantum mechanics.

It turns out, as we have already indicated, that in order to reproduce the usual mathematical formalism of quantum mechanics (i.e. the Schrödinger equations and the transformation functions etc.) we will not need a complete set of deterministic laws governing particle motions but will instead need to claim only certain general properties of those motions (including for example that orbital motions are continuous and that orbital motions in the *present* are never affected by the values of inter-particle potentials in the *future*). Assuming only such general properties we will find that the usual Schrödinger equations and the usual transformation functions (like those connecting wave functions in the position and momentum representations) can be deduced using the new probability theory.*

Taking the usual quantum mechanical equations as a guide we are thus led to formulate (the simplest possible) physical laws (and the simplest possible laws of complex-valued probability theory) which will give those same equations. In one sense nothing new is achieved – no new testable predictions will be given in this work. But a clear distinction will be drawn between the physical world and our knowledge of it, and physical laws will be revealed that previously lay hidden. Our interpretation of quantum mechanics may therefore seem clearer than previous interpretations.

* Note however that the usually arbitrary constant phase factors in transformation functions sometimes have definite (known) values in our theory.

CHAPTER I

THE LAWS OF COMPLEX-VALUED PROBABILITY

1. Knowledge and observation

In quantum mechanics measurements designed to reveal the truth values of particular propositions claiming dynamical properties of the physical world may change the truth values of other such propositions and do so in a way that (by the uncertainty principle) cannot always be controlled or predicted.*

However, a measurement may leave unchanged the truth values of *some* propositions claiming dynamical properties. We shall say that such a measurement is ‘harmless’ with regard to those properties and with regard to the propositions claiming them.

Preparation of a quantum mechanical system may be conducted to ensure that a specified physical property of that system is present. But as a result of such preparation it may sometimes be that other physical properties necessarily come to be present also even though these properties need not naturally occur along with the property we prepared. This is another way in which the uncertainty principle prevents us from preparing or knowingly realising *any* possible physical state of a quantum mechanical system.

In formulating quantum mechanics we will be building a kit for constructing models (mental images) of processes in the physical world. But, because of the uncertainty principle, it will be necessary also to model our states of *knowledge* of dynamical properties and we will need to formulate the possible states of this knowledge over time.†

Henceforth, unless otherwise stated, we will mean by ‘the physical world’ our model of any process in it and by ‘knowledge’ knowledge supposed to be held in relation to the ‘physical world’ which will always include a model of the quantum mechanical system under study and may sometimes include a model of measuring or detecting apparatus occasionally in interaction with the quantum mechanical system.

* With regard to any quantum mechanical system under consideration during a time period we will assume we are aware of all processes of observation of that system and the times they are carried out so we will not have to consider the possibility and probability of other observers conducting measurements without our knowledge. We will not necessarily need to know the results of the measurements conducted but we will always suppose we know the exact *nature* and *time* of the measurements.

† This differs from the situation in classical physics (including relativity) where acquisition of knowledge ideally has no physical effects and the exact values of any combination of dynamical properties are assumed to be *harmlessly* observable in principle (even if exactly how this could be done is often not immediately obvious). Later, when the present interpretation of quantum mechanics is developed to a certain degree, we will be able to model measurements - processes that lead to (directly observable) macroscopic images of microscopic aspects - and so demonstrate the possibility of acquiring knowledge of certain dynamical properties of the quantum world in a manner entirely consistent with the claims of the quantum theory itself (see Chapter XIII).

In our theory of probability and its applications the propositions we employ are of three types. Those of type 1 claim specific dynamical properties of the physical world.* Those of type 2 claim unchanging properties of the physical world.† Those of type 3 claim laws of quantum mechanics, laws of the (new) probability theory etc.

Any knowledge is expressed by marking certain propositions as *true*. We will thus speak of knowledge of three kinds according respectively to the type of propositions used to express it. Our whole knowledge will be a combination of knowledge of all three kinds. Only knowledge of the first kind is subject to the uncertainty principle.

We will often denote by X (but sometimes by A or B , etc) a proposition whose probability is sought. This will always be a proposition of the first type because the probabilities of dynamical properties are the main thing to be calculated in quantum mechanics.‡

We will denote most often by Y a proposition representing our knowledge of the first kind (our knowledge of dynamical properties of the physical world).

We will denote by G a (very long!) proposition representing our ‘general knowledge’. This includes our knowledge of the third kind (our knowledge of the laws of quantum mechanics and of the probability theory etc) and our knowledge of the second kind (our knowledge of the unchanging properties of the physical world).

We denote the probability of X knowing Y and G by $\Phi(X|YG)$ (the product YG representing the conjunction of Y and G).

2. General rules of probability and propositional logic

2.1 Complex-valued probabilities

When a probability $\Phi(X|YG)$ exists, its squared modulus $|\Phi(X|YG)|^2$ is our degree of belief in X knowing Y and G , and its argument or phase $\angle\Phi(X|YG)$ (defined modulo 2π) is our ‘phase of belief’ in X knowing Y and G . Both degrees of belief and phases of belief are dimensionless. If only the modulus $|\Phi(X|YG)|$ of a probability $\Phi(X|YG)$ is calculable we say the probability is ‘determinate to within a phase’ or that its phase is ‘indeterminate’.

Henceforth our general knowledge G (when common to all knowledge with respect to which probabilities are calculated and common to all reasoning) will always be assumed but not referred to explicitly in the algebra. For example we will denote our

* E.g. that the particles in our model lie in specified regions of space at a particular time.

† E.g. that the particles taking part in our model have certain masses (perhaps large or theoretically infinite in the case of the particles employed in our modelling of any macroscopic apparatus) and that a certain formula for the inter-particle potential energy of the particles applies. (Knowledge of this kind is not subject to the uncertainty principle.)

‡ The probability theory developed here could (perhaps with little or no modification) be applied to the calculation of probabilities of propositions of the second type also when we are uncertain of some unchanging properties of the physical world (e.g. the number of particles making up a system). However in the interest of simplicity of the formulation of the theory we do not discuss such applications in the present monograph.

knowledge as Y not as YG , we will write $\Phi(X|YG)$ simply as $\Phi(X|Y)$, and $YG \Rightarrow X$ simply as $Y \Rightarrow X$. The symbols \Rightarrow , \Leftarrow and \Leftrightarrow are always used in this monograph to indicate implication *by reasoning*. They are not used merely to indicate pure logic relations between the truth values of propositions. However, we will explain soon how implication in the sense we use it will generally need to be quantified by a phrase.

Starting with supposed knowledge Y of the dynamical properties of a quantum mechanical system, further knowledge A might be learnt (by measurement) without invalidating our original knowledge Y . Having acquired such further knowledge A , our probability for a proposition X claiming a dynamical property of the quantum mechanical system generally changes from $\Phi(X|Y)$ to $\Phi(X|AY)$, where the conjunction AY expresses our new state of knowledge. With regard to the future, the effect of acquiring knowledge A may be to render redundant all or part of our original knowledge Y . The acquisition of the further knowledge A might be accomplished without changing the truth values of propositions X_i claiming *certain* dynamical properties of the quantum mechanical system.* It may nonetheless affect *our probabilities* for the X_i just as new knowledge does in classical Bayesian probability theory and it may of course affect the *truth or falsity* of other propositions on account of the uncertainty principle.

Dynamical properties may be *physically* compatible with one another (i.e. all be present) but be nonetheless termed ‘compatible’ or ‘incompatible’ according to the possibility or impossibility (on account of the uncertainty principle) of us *knowing* of the presence of them all.

Because of the uncertainty principle we cannot know the truth or falsity of a proposition claiming ‘incompatible’ dynamical properties.† And, while we are in a state of knowledge (pure or not), we cannot speak of *probabilities* of propositions making claims relating to two or more ‘incompatible’ dynamical properties‡; such probabilities do not exist.§

In contrast, the uncertainty principle never in itself prevents us from knowing the truth or falsity of propositions claiming ‘compatible’ dynamical properties. And we can

* The subscript i (not to be confused with $\sqrt{-1}$) denotes a parameter (taking one of a number of possible values e.g. one or other integer $i = 1, \dots, n$) used to label the propositions of a certain class. This convention (with the use of various subscripts i, j, \dots) applies throughout the monograph.

† For example we cannot know the truth of a proposition claiming a precise position *and* a precise momentum of a particle in the present or at some future time because those properties are ‘incompatible’. (Note however that *retrospective* knowledge of the truth or falsity of a proposition claiming such properties is sometimes a possibility -see section 2.3 of Chapter XV.)

‡ So, for example, because precise position *and* precise momentum of a particle are ‘incompatible’ properties, there are no joint probability distributions pertaining to those properties in the present or in the future.

§ But if a probability of a proposition X (claiming dynamical properties) exists, this does not guarantee that the truth or falsity of X could in principle be known. We may not be able to acquire knowledge of the truth (or falsity) of X for some reason unconnected with the uncertainty principle. For example, X might be a proposition of an ‘improper basis’ (see section 1 of Chapter X).

always speak of probabilities of such propositions based on our knowledge (pure or not). Even though those probabilities may be wholly or partly *indeterminate*, they do *exist*.

The distinction between compatible and incompatible properties will play an important part in our interpretation of quantum mechanics.

2.2 Laws concerning implication, characteristic phases and extreme values of probability

2.2.1 Implication and characteristic phases

The nature of implication in quantum mechanics and complex-valued probability is somewhat different from its nature in classical physics and classical probability. An implication is now quantified by a ‘phase’, by a (dimensionless) number denoted α , β or γ ...etc, taking a real value defined modulo 2π . With regard to any propositions A and B claiming dynamical properties of the physical world, if under our general knowledge G alone proposition A implies proposition B , i.e. if the truth of A entails the truth of B we may write this as $A \Rightarrow^\gamma B$ meaning A implies B with phase γ . When consideration of the phase is unimportant we simply write $A \Rightarrow B$.

A relation between phases of implication and phases of belief will be postulated in section 2.2.2. This relation will (by the laws of probability) give or suggest general rules for phases of implication.* There is therefore no need to formulate all these rules independently. We claim the general rule

$$A \Rightarrow^0 A \tag{2.2.1.1}$$

i.e. that any proposition implies itself with zero phase of implication, and the general rule of phase addition, that

$$\text{if } A \Rightarrow^\alpha B \text{ and } B \Rightarrow^\beta C \text{ then } A \Rightarrow^{\alpha+\beta} C. \tag{2.2.1.2}$$

Phases of implication (like phases of belief) may be calculable or may be indeterminate.

We say A and B are ‘equivalent’ (written $A \Leftrightarrow B$ or more fully as $A \stackrel{-\alpha}{\Leftrightarrow}^\alpha B$) if (under knowledge G) $A \Rightarrow^\alpha B$ and $B \Rightarrow^{-\alpha} A$ whether the phase of implication α is determinate or not and if determinate whatever it may be.† So

$$A \Leftrightarrow B \text{ is the same as } \{ A \Rightarrow^\alpha B \text{ and } B \Rightarrow^{-\alpha} A \}. \tag{2.2.1.3}$$

We say A and B are ‘fully equivalent’ (denoted $A \equiv B$ or $A \stackrel{0}{\Leftrightarrow} B$) if and only if the phases of implication are zero. So

* For example rules (2.2.1.2), (2.2.1.3) and the first of (2.2.1.7) are suggested by results (10.1.11), (10.1.10) and (10.3.1) of Chapter II respectively.

† On account of (2.2.1.1) and (2.2.1.2), under equivalence, the phase with which A implies B must clearly be equal and opposite to that with which B implies A .

$$A \equiv B \text{ is the same as } \{ A \Rightarrow^0 B \text{ and } B \Rightarrow^0 A \}. \quad (2.2.1.4)$$

The existence of phases of implication generalises the character of natural laws in that we might now include a form of natural law in which possession of one property implies possession of another *with a specified phase* α .^{*} However, although it would simplify the derivation of some transformation functions, we do not adopt this generalisation in its full form as there seems to be no actual need for it. In the formulation of natural laws we will however often specify that one property implies another with a phase of implication equal to (or expressly *unequal* to) zero.[†]

Any two propositions A and B that *plainly* claim states that are *physically identical* on account of our general knowledge imply one another with zero phases of implication.^{‡§}

The usual logical laws of idempotence, commutation, association, distribution, duality and double negation are taken to hold in the sense that for any propositions A, B, C and D :^{**}

$$\left. \begin{aligned} AA &\Leftrightarrow A, & A+A &\Leftrightarrow A; \\ AB &\Leftrightarrow BA, & A+B &\Leftrightarrow B+A; \\ A(BC) &\Leftrightarrow (AB)C, & A+(B+C) &\Leftrightarrow (A+B)+C; \\ A(B+C) &\Leftrightarrow AB+AC, & A+BC &\Leftrightarrow (A+B)(A+C); \\ \text{If } C &\Leftrightarrow AB \text{ then } \bar{C} &\Leftrightarrow \bar{A}+\bar{B}, & \text{and if } D &\Leftrightarrow A+B \text{ then } \bar{D} &\Leftrightarrow \bar{A}\bar{B}; \\ \bar{\bar{A}} &\Leftrightarrow A \end{aligned} \right\} \quad (2.2.1.5)$$

* This generalisation seems possible at least if the phases are specified only to within an indeterminate sign i.e. specified as $\pm \alpha$ with α given; the possibility of wave function conjugation (see section 8) being then maintained.

† See, for example, the law of constancy of momentum under coordinate displacement (section 1 of Chapter VI).

‡ For example if A = 'particle is at \mathbf{r} in \mathbf{O} ' and B = 'particle is at \mathbf{r}' in \mathbf{O}' ' (\mathbf{O} and \mathbf{O}' being fixed coordinate frames and \mathbf{r} and \mathbf{r}' position vectors in those frames representing the same point \mathbf{P} in fixed space, then $A \overset{0}{\Leftrightarrow} B$. On the other hand if A and B claim equal values of different dynamical properties (that are only dimensionally the same) then it might be that $A \overset{-\lambda}{\Leftrightarrow} B$ where $\lambda \neq 0$. Sameness and equality are after all quite different things.

§ Note that if propositions A and B claim things that are physically identical it is still possible that they are not fully equivalent. This can happen when those propositions are expressed in different (but equivalent) logical ways. If for example $A \overset{0}{\Leftrightarrow} B$ then because A and AA may not be fully equivalent AA and B may not be fully equivalent (and $AA+A$ and B may not be fully equivalent either). This is why we state that $A \overset{0}{\Leftrightarrow} B$ when A and B *plainly* claim things that are physically identical. The term *plainly* indicates that the propositions do not involve unnecessary conjunctions and disjunctions. Unless otherwise stated we will assume propositions are always stated *plainly*.

** When we write a conjunction (such as AB or $A(B+C)$, ... etc.) we imply that the conjunction *exists*, i.e. that the members of the conjunction are not mutually exclusive.

where (as in [2]) $+$ denotes disjunction, a simple product denotes conjunction and a bar denotes negation. But the equivalence in these laws is not always *full* equivalence. The cases in which full equivalence always applies are:

$$\left. \begin{aligned} A + A &\stackrel{0}{\Leftrightarrow} A; \\ AB &\stackrel{0}{\Leftrightarrow} BA, \quad A + B \stackrel{0}{\Leftrightarrow} B + A; \\ A(BC) &\stackrel{0}{\Leftrightarrow} (AB)C, \\ A + (B + C) &\stackrel{0}{\Leftrightarrow} (A + B) + C \text{ when } A, B \text{ and } C \text{ are mutually exclusive;} \\ \overline{\overline{A}} &\stackrel{0}{\Leftrightarrow} A. \end{aligned} \right\} (2.2.1.6)$$

Note the qualification in the last but one case of (2.2.1.6).

In addition to (2.2.1.1) and (2.2.1.2) we also claim the following rules of phases of implication under conjunction and disjunction:

$$\left. \begin{aligned} \text{If } A \Rightarrow^\alpha C \text{ and } B \Rightarrow^\beta D \text{ then } AB \Rightarrow^{\alpha+\beta} CD, \\ \text{If } A \Rightarrow^\alpha C \text{ and } B \Rightarrow^\beta D \text{ then } A + B \Rightarrow^\gamma C + D \end{aligned} \right\} (2.2.1.7)$$

where the phase of implication γ is generally indeterminate.

Note that with regard to our general knowledge (which includes knowledge of the unchanging properties of the physical world) if G' and G'' are propositional expressions of all (or a part) of that general knowledge and if $G' \Rightarrow G''$ then $G' \Rightarrow^0 G''$ always holds, and if G' and G'' are equivalent, they are always fully equivalent, i.e. $G' \stackrel{0}{\Leftrightarrow} G''$.

In our new probability theory and new propositional logic, as well as phases of belief and phases of implication, there are (generally indeterminate) *characteristic* phases.

In relation to any proposition A claiming a dynamical property of the physical world and any other such proposition Y which could represent a state of knowledge of the physical world, there corresponds a phase, denoted $\text{ch}(A|YG)$, characteristic of A under knowledge YG , and corresponding to Y there is a phase, denoted $\text{ch}(YG)$, characteristic of knowledge YG . As usual, when our general knowledge G is common to all our reasoning we will avoid reference to it and just as we write $\Phi(X|YG)$ as $\Phi(X|Y)$ we will write $\text{ch}(A|YG)$ as $\text{ch}(A|Y)$, and $\text{ch}(YG)$ as $\text{ch}(Y)$. Any probability $\Phi(A|Y)$ can always be written as

$$\Phi(A|Y) = \sqrt{|\Phi(A|Y)|^2} e^{i(\chi-k)} \quad (2.2.1.8)$$

where

$$\left. \begin{aligned} \chi &= \text{ch}(A|Y) \\ k &= \text{ch}(Y) \end{aligned} \right\} \quad (2.2.1.9)$$

So our phase of belief in A knowing Y is the difference $\chi - k$ between the phase characteristic of A under knowledge Y and the phase characteristic of knowledge Y . And we claim that χ remains the same under an equivalence transformation of Y , i.e.

$$\text{ch}(A|Y) = \text{ch}(A|Y') \quad \text{whenever} \quad Y \stackrel{-\lambda}{\Leftrightarrow} Y'. \quad (2.2.1.10)$$

In the special case Y represents no knowledge whatsoever of the dynamical properties of the physical world (we denote this knowledge by Y_0 and under it we have knowledge (in G) only of the unchanging properties of the physical world) the phase characteristic of our knowledge is zero, i.e.

$$\text{ch}(Y_0) = 0. \quad (2.2.1.11)$$

Then, in (2.2.1.8), $k = 0$, and our phase of belief in A equals χ (or $\text{ch}(A|Y_0)$) and is the phase $\text{ch}(A|G)$ characteristic of A under knowledge G alone. So we can write $\Phi(A|Y_0)$ as

$$\Phi(A|Y_0 G) = \Phi(A|G) = \sqrt{|\Phi(A|G)|^2} e^{i \text{ch}(A|G)} \quad (2.2.1.12)$$

If \tilde{G} is any proposition claiming a dynamical property of the physical world but one *necessarily true* under our general knowledge G ,* and if our knowledge Y of dynamical properties is expressed as $\tilde{G}Y$, then the phase characteristic of knowledge $\tilde{G}Y$ is the same as that of Y , and $\tilde{G}Y$ and Y are fully equivalent:

$$\text{ch}(\tilde{G}Y) = \text{ch}(Y), \quad (2.2.1.13)$$

$$\tilde{G}Y \stackrel{0}{\Leftrightarrow} Y \quad (2.2.1.14)$$

Also, we claim

$$\text{ch}(\tilde{G}) = 0 \quad (2.2.1.15)$$

and

* For example \tilde{G} might claim that at a particular time a particle occupies one or other of the infinitesimal volume elements filling all space.

$$\text{ch}(\tilde{G}|Y) = 0. \quad (2.2.1.16)$$

And because of (2.2.1.16) we have from (2.2.1.8) that

$$\Phi(\tilde{G}|Y) = e^{-ik} \quad (2.2.1.17)$$

where k is the phase characteristic of knowledge Y .

We note some further rules as follows.

As noted already in (2.2.1.6) we assume, for any proposition A , that

$$A + A^0 \Leftrightarrow^0 A \quad (2.2.1.18)$$

but in the undoubtedly true equation

$$AA^{-\alpha} \Leftrightarrow^{\alpha} A \quad (2.2.1.19)$$

α is generally different from zero.

And if, under our general knowledge G , $A \Rightarrow Y$ and Y represents a possible state of knowledge of dynamical properties of the physical world then (under G) we claim

$$A^{-k} \Leftrightarrow^k AY \quad (2.2.1.20)$$

where k is the phase characteristic of knowledge Y .^{*} And we claim the unidirectional implication

$$AY \Rightarrow^{-k} A \quad (2.2.1.21)$$

is valid generally (with k equal to the phase characteristic of knowledge Y) whether or not $A \Rightarrow Y$.

We also claim the following law:

Constancy of the phase of implication between disjunctions of similarly equivalent but not exhaustive propositions

If propositions A, B, \dots are not exhaustive and no two are equivalent, and if propositions A', B', \dots are related to them through the same phase α of implication (so that $A^{-\alpha} \Leftrightarrow^{\alpha} A', B^{-\alpha} \Leftrightarrow^{\alpha} B', \dots$), then the phase of equivalence of $A + B + \dots$ and $A' + B' + \dots$ is also α , (i.e. $A + B + \dots^{-\alpha} \Leftrightarrow^{\alpha} A' + B' + \dots$).

^{*} This rule is employed in the derivation of a wave function after harmless conditioning (section 4 of Chapter II).

Finally we claim the following *law of substitution*, that if, under our general knowledge, $A \overset{0}{\Leftrightarrow} B$, then in any logical formula involving A (e.g. $A + D \Rightarrow^\alpha C$) B may be substituted for A (giving in our example $B + D \Rightarrow^\alpha C$) and the formula will remain as valid as it was before.

In Appendix I we set up an (extended) Venn diagram to visualise propositions, phases of implication and phases characteristic of knowledge by relating them to geometrical features in the diagram. This helps us to appreciate the feasibility of these concepts and the consistency of the purely logical laws claimed in relation to them, upon which the present theory of complex-valued probability (with the concepts of degrees of belief, phases of belief and phases characteristic of propositions under knowledge) is developed.

2.2.2 Extreme values of probability and ‘logical expectation’

In the following three laws concerning extreme values of a probability $\Phi(X|YG)$, propositions X and Y are, as usual, propositions claiming dynamical properties of the physical world, G is our general knowledge and \bar{X} stands for ‘not X ’. The laws are more involved than the laws of extreme values in classical probability because of the existence of phases of implication.

First law If (under G) proposition Y implies proposition X (i.e. if $Y \Rightarrow^\alpha X$) with a determinate or indeterminate phase α , then $\Phi(X|Y) = e^{i\alpha}$. If (under G) only the *acquisition* of knowledge Y is known to *physically* bring about or ensure the truth of X then $\Phi(X|Y) = e^{i\alpha}$ where α is an indeterminate phase. Conversely, if $\Phi(X|Y) = e^{i\alpha}$ where α is a *determinate* phase we can claim $Y \Rightarrow^\alpha X$ (so X is a necessary consequence of Y whether or not we hold knowledge of the truth of Y).^{*} But if $\Phi(X|Y) = e^{i\beta}$ where β is an *indeterminate* phase we can claim only that we *expect* X to be true under knowledge Y .

So if (under G) Y implies X with some phase of implication, our degree of belief in X under knowledge Y is equal to 1 and our phase of belief in X under knowledge Y is always equal to the phase of implication of X by Y . In particular, since any proposition implies itself with zero phase of implication we always have $\Phi(Y|Y) = 1$. But given $\Phi(X|Y) = e^{i\beta}$ where β is indeterminate we are led only to *expect* the truth of X ; it may be (i) that $Y \Rightarrow^\beta X$ (i.e. that X is a necessary consequence of Y whether or not we hold knowledge of the truth of Y) or (ii) only the uncontrollable physical effect of the

^{*} Note that probabilities are not the same as truth values so a probability $\Phi(X|Y) = e^{i\alpha}$ is not the truth value of X knowing Y . The (pure logic) law of bivalence (or the principle of the excluded middle) is not therefore contradicted here on account of the variety of possible values of α .

acquisition of knowledge Y brings about or ensures the truth of X . Without further information we cannot tell if (i) or (ii) applies. And it may be that neither do, in which case $\Phi(X|Y) = e^{i\beta}$ (β indeterminate) does not indicate the *certainty* of X under knowledge Y but (iii) only the *logical expectation* of X under knowledge Y .*

Second law If (under G) $Y \Rightarrow \bar{X}$ with a determinate or indeterminate phase, or if we know that acquisition of knowledge Y physically brings about or ensures the falsity of X , then $\Phi(X|Y) = 0$. Conversely given $\Phi(X|Y) = 0$, we may claim only that we *expect* X to be false under knowledge Y .

So given $\Phi(X|Y) = 0$ it might be (i) that $Y \Rightarrow \bar{X}$ (i.e. that X is a necessarily false on account of Y whether or not we hold knowledge of the truth of Y) or (ii) it is the physical acquisition of knowledge Y that brings about or ensures the falsity of X . Without further information we cannot tell if (i) or (ii) applies. And it may be that neither do, in which case $\Phi(X|Y) = 0$ does not indicate the *certainty* that X is false under knowledge Y but only the *logical expectation* that X is false under knowledge Y .†

Third law If we expect the truth (or the falsity) of X knowing Y , or if we are certain of the truth (or the falsity) of X knowing Y , then $|\Phi(X|Y)|^2 = 1$ (or $|\Phi(X|Y)|^2 = 0$). In all other cases $0 < |\Phi(X|Y)|^2 < 1$.

With regard to logical expectation we claim the following law in which proposition Y represents our state of knowledge and the propositions X_i $i = 1, 2, \dots$ claim dynamical properties existing at times after the time of acquisition of our knowledge Y .

Law of logical expectation of a conjunction and disjunction

Suppose under knowledge Y (pure or not) we logically expect the truth of X_1 and we logically expect the truth of X_2 . Then so long as X_1 and X_2 refer to compatible properties we can claim to logically expect the truth of both the

* So when we ‘expect X to be true’ (i), (ii) or (iii) applies. But note that in our new logic there is a difference between certainty (as in cases (i) and (ii)) and *logical expectation* (as in case (iii)). Certainty implies logical implication or physical causation. But logical expectation is unsubstantiated belief. Importantly (and remarkably) however, it seems to be the case that expectations under *pure* knowledge are borne out in quantum mechanics virtually every time they are tested experimentally even when we are sure that logical implication and/or physical causation are not the reason. (If the truth of X is only ensured by the *acquisition* of knowledge Y or if the truth of X is only *expected* under knowledge Y we do not write $Y \Rightarrow X$. We reserve \Rightarrow , \Leftarrow and \Leftrightarrow for implications which apply (by the laws of nature or of logic) independently of any knowledge we may hold of the dynamical properties of the physical world.)

† That we cannot claim for certain (under knowledge Y) that X is false just because $\Phi(X|Y) = 0$ seems to be related to the fact that the phase of the complex number zero is indeterminate.

disjunction $X_1 + X_2$ and the conjunction $X_1 X_2$. But if X_1 and X_2 refer to *incompatible* properties we can claim to logically expect the truth of the disjunction $X_1 + X_2$ but we cannot claim to logically expect the truth of the conjunction $X_1 X_2$.*

2.2.3 The variability of the absolute phase of probabilities under given knowledge

Because of the existence of phases of implication we need to give consideration to the form of the proposition Y representing our knowledge of dynamical properties of the physical world. If Y and Y' express essentially the same state of knowledge because they are equivalent, i.e. if $Y \stackrel{-\lambda}{\Leftrightarrow} Y'$ under G , the probabilities $\Phi(X|Y)$ and $\Phi(X|Y')$ for a proposition X claiming a dynamical property of the physical world generally differ in phase. But we assume, as a general law, that the phase of $\Phi(X|Y')$ differs from the phase of $\Phi(X|Y)$ by the same amount whatever the proposition X . Letting X_j stand for the general proposition about a dynamical property we therefore have

$$\Phi(X_j|Y') = \Phi(X_j|Y)e^{i\alpha} \quad (2.2.3.1)$$

where α is independent of j .

On putting $X_j = Y$, (2.2.3.1) gives $\Phi(Y|Y') = e^{i\alpha}$ since $\Phi(Y|Y) = 1$. Similarly on putting $X_j = Y'$ in (2.2.3.1) we obtain $\Phi(Y'|Y) = e^{-i\alpha}$. Therefore, by the first law of extreme values of probability, the phase α in (2.2.3.1) is -1 times the phase of implication λ in the supposed relation $Y \stackrel{-\lambda}{\Leftrightarrow} Y'$; i.e. $\alpha = -\lambda$.

Thus the *relative* phases of the $\Phi(X_j|Y)$ remain unchanged under an equivalence transformation of Y and it is these relative phases and the absolute values of the moduli $|\Phi(X_j|Y)|$ that characterise the probabilities of the X_j in relation to one another. The *absolute* phases are indicative of the manner in which we express the knowledge upon which we base our probabilities.

* This is related to the fact that joint probabilities (like $\Phi(X_1 X_2|Y)$) of the propositions X_1 and X_2 claiming incompatible properties under knowledge Y do not exist (see toward the ends of sections 2.1 and 3.2). So we may calculate that $\Phi(X_1|Y) = e^{i\alpha}$ (α indeterminate) and that $\Phi(X_2|Y) = e^{i\beta}$ (β indeterminate), but be unable to show that $\Phi(X_1 X_2|Y) = e^{i\gamma}$ (γ indeterminate) because $\Phi(X_1 X_2|Y)$ does not exist. (Note that the product rule (2.4.1) cannot give us a value for $\Phi(X_1 X_2|Y)$ because a necessary condition for applying that rule (namely that X_1 and X_2 claim compatible dynamic properties) is not met.) The *law of expectation of a conjunction and disjunction* will be of use in resolving paradoxes arising from Bell type theorems (see sections 2 and 3 of Chapter XV).

2.3 The sum rule of probability

The sum rule for the probability of disjunctions of propositions claiming dynamical properties of the physical world under knowledge Y is as follows.

Sum rule Under knowledge Y , if propositions A and B are mutually exclusive, the probability of their disjunction is always given by

$$\Phi(A + B|Y) = e^{i(\chi-k)} \sqrt{|\Phi(A|Y)|^2 + |\Phi(B|Y)|^2} \quad (2.3.1)$$

where k is the phase characteristic of knowledge Y and χ the phase characteristic of the disjunction $A + B$ under knowledge Y . Generally k is indeterminate and χ is indeterminate. And χ cannot be expressed as a universal function of the individual phases characteristic of A and B under knowledge Y .

But, as in classical probability, our *degree of belief* in ‘ A or B ’ (when A and B are mutually exclusive) is evidently the sum of our *degrees of belief* in A and B separately.

Note that (2.3.1) generalises to

$$\Phi(A + B + \dots|Y) = e^{i(\eta-k)} \sqrt{|\Phi(A|Y)|^2 + |\Phi(B|Y)|^2 + \dots} \quad (2.3.2)$$

for any finite number m of mutually exclusive propositions A, B, \dots ; k being the phase characteristic of knowledge Y , and η the phase characteristic of the disjunction $A + B + \dots$ under knowledge Y (η being generally indeterminate, and not a universal function of the individual phases characteristic of A, B, \dots under knowledge Y).

Now $G \Rightarrow X_1 + \dots + X_n$ whenever propositions X_i ($i = 1, \dots, n$) claiming dynamical properties are mutually exclusive *and* exhaustive under our general knowledge G . Then, by (2.2.1.16) or (2.2.1.17) it must be that in (2.3.2) (with A, B, \dots replaced by X_1, X_2, \dots, X_n) the characteristic phase η is zero, so we have

$$\Phi(X_1 + \dots + X_n|Y) = e^{-ik}, \quad \text{and} \quad \sum_{i=1}^n |\Phi(X_i|Y)|^2 = 1 \quad (2.3.3)$$

whenever X_1, X_2, \dots, X_n are mutually exclusive and exhaustive.

2.4 The product rule of probability

There is also a product rule for the probability of conjunctions of propositions claiming dynamical properties of the physical world. It contains a qualification to guard against the uncertainty principle.

Product rule The probability of a conjunction AB is given by

$$\Phi(AB|Y) = \Phi(A|Y)\Phi(B|AY)e^{i(k+\varepsilon)} \quad (2.4.1)$$

where k and ε are the phases characteristic of knowledge Y and of knowledge A respectively and are generally indeterminate. But (2.4.1) holds only when A and B claim compatible properties and when A is a possible state of knowledge that can be held on its own or in combination with knowledge Y .*

So, under the right conditions we have, as in classical probability, that under any knowledge Y our *degree of belief* in AB is the product of our *degree of belief* in A under knowledge Y and our *degree of belief* in B under knowledge AY .

We note that (2.4.1) generalises to

$$\begin{aligned} \Phi(A_1 A_2 A_3 \dots A_m | Y) = & \Phi(A_1 | Y) \Phi(A_2 | A_1 Y) \Phi(A_3 | A_1 A_2 Y) \dots \Phi(A_m | A_1 \dots A_{m-1} Y) \\ & e^{i(k(m-1) + (m-1)\varepsilon_1 + (m-2)\varepsilon_2 + \dots + \varepsilon_{m-1})} \end{aligned} \quad \dots(2.4.2)$$

where $k, \varepsilon_1, \varepsilon_2, \dots, \varepsilon_{m-1}$ are the phases characteristic of knowledge $Y, A_1, A_2, \dots, A_{m-1}$ respectively (and are generally indeterminate), A_1, A_2, \dots, A_m claim compatible properties, and A_1, A_2, \dots, A_{m-1} are possible states of knowledge that can be held on their own or in combination with knowledge Y .

And with regard to phases characteristic of knowledge we assume the following general rule:

First addition rule for phases characteristic of knowledge

If Y_1, \dots, Y_n are n propositions representing n possible and compatible states of knowledge, then the phase κ characteristic of the state of knowledge $Y_1 \dots Y_n$ is the sum of the phases $\kappa_1, \dots, \kappa_n$ respectively characteristic of Y_1, \dots, Y_n .

* Note that in classical probability applied to classical mechanics, as long as $\Phi(A|Y) \neq 0$ the conjunction AY of propositions claiming dynamical properties always represents a possible state of knowledge unambiguously. But in complex-valued probability applied to quantum mechanics this is not generally so because knowledge of A and knowledge of Y may be incompatible on account of the uncertainty principle. Note also that (2.4.1) is formally correct even when $\Phi(A|Y) = 0$ i.e. even when, under Y , proposition A is expected to be false. For although $\Phi(B|AY)$ may now be indeterminate (since AY may not now represent a possible state of knowledge) the RHS of (2.4.1) is zero and the LHS is zero also since A (and therefore AB) is expected to be false under knowledge Y .

2.5 Independence

There are three ways in which the first of two propositions A and B claiming dynamical properties of the physical world can be independent of the second.

Causal independence

A is ‘causally independent’ of B when the truth value of B (whatever it is) does not determine the truth value of A through *direct physical* causality.*

Cognitive independence

A is ‘cognitively independent’ of B when we can acquire (by measurement) the truth value of B without affecting the truth value of A .†

Logical independence

A is ‘logically independent’ of B under knowledge Y if and only if

$$\Phi(AB|Y) = \Phi(A|Y)\Phi(B|Y)e^{ik} \quad (2.5.1)$$

where k is the (generally indeterminate) phase characteristic of knowledge Y . It follows that if A is ‘logically independent’ of B under knowledge Y then B is ‘logically independent’ of A under knowledge Y .

The definition of logical independence generalises in the following way. Any finite number m of propositions A_1, A_2, \dots, A_m are ‘logically independent of each other’ under knowledge Y if and only if

$$\Phi(A_1 A_2 \dots A_m | Y) = \Phi(A_1 | Y) \Phi(A_2 | Y) \dots \Phi(A_m | Y) e^{ik(m-1)} \quad (2.5.2)$$

where k is the phase characteristic of knowledge Y . And whenever A_1, A_2, \dots, A_m are logically independent of each other under knowledge Y , any conjunction of them (e.g. $(A_1 A_2)$) is logically independent (under knowledge Y) of any of the remaining A_i and of any conjunction formed from them.

Causal and logical independence are thus defined in a manner the same as or very similar to the way they are defined in classical probability. But cognitive independence is new – special to complex-valued probability on account of the uncertainty principle. In the classical limit, i.e. under conditions in which classical and complex-valued probability

* If the truth value of A and the truth value of B are only related indirectly through a *common* cause, A and B are still causally independent of one another.

† It is of course nonsensical to claim A is cognitively independent of B when acquisition of the knowledge of the truth or falsity of B is not possible.

theory coexist (see section 6) cognitive independence is always present – it holds for any pair of propositions.

Causal (or cognitive) independence is present or not present as a matter of fact regardless of the specific knowledge Y we may hold of dynamical properties. But logical independence may be present under some states of knowledge Y and not present under others.

The three kinds of independence are quite different. Knowledge of one kind of independence does not generally imply knowledge of another.*

2.6 Sample spaces

We will use the term ‘sample space’ to denote a set of propositions claiming dynamical properties of part of the physical world over a period of time. These include atomistic propositions[†], disjunctions of them, (non-empty) conjunctions of the disjunctions and negations, all representable in a Venn diagram[‡]. Though we may not know which, one of the atomistic propositions of a sample space is supposed to be true while all the others are false.

Knowledge in relation to a sample space S need not be knowledge of the truth of a proposition of S , it can be knowledge of the truth of any proposition which can influence our assignment of probabilities to the propositions of S .

As in classical probability theory, a proposition can be a member of more than one sample space but it can only have one probability given our knowledge.

Sample spaces that have no propositions in common will be called ‘separate’.

Independent sample spaces

Sample spaces may be independent of each other in three different ways.[§] They must first of all be separate and then they are ‘causally’, ‘cognitively’ or (under certain knowledge) ‘logically’ independent according as all the propositions of any one of the sample spaces are causally, cognitively or logically independent of all the propositions^{**} of the others.

*It may be that logical independence is not possible without cognitive independence. But we will see, for example, that the propositions ‘ $\sigma = \frac{1}{2}$ ’ and ‘ $\sigma' = \frac{1}{2}$ ’ claiming particular values of the z components of spin σ and σ' of an electron in fixed coordinate systems O and O' whose z axes are not parallel, are *causally* independent but not *cognitively* independent.

In the case of coexistence of classical and complex-valued probability (see section 6) we know cognitive independence is always present but this does not imply knowledge of causal or logical independence and knowledge of causal independence does not imply knowledge of logical independence or vice versa (see page 92 of [2]).

[†] those that cannot be expressed as disjunctions of propositions of the sample space

[‡] We mean here a *classical* Venn diagram. (We are not referring to the extended Venn diagram set up in Appendix I).

[§] In applications, which sample spaces qualify as independent (or dependent) in any one of the three ways listed will sometimes be declared (axiomatically) as being part of our general knowledge.

^{**} For the purpose of defining cognitive independence of sample spaces we need refer only to those propositions of the sample spaces whose truth or falsity could in principle be learnt.

Combinations of sample spaces

Suppose we have two separate sample spaces $S^{(1)}$ and $S^{(2)}$. Then, as in classical probability theory, we can consider them combined together as one sample space $S^{(1)}S^{(2)}$ ($S^{(1)}S^{(2)}$ and $S^{(2)}S^{(1)}$ being equivalent). Each atomistic proposition of $S^{(1)}S^{(2)}$ is, as usual, the conjunction of an atomistic proposition of $S^{(1)}$ and an atomistic proposition of $S^{(2)}$. This can be repeated any number of times to form sample spaces $S^{(1)}S^{(2)}S^{(3)}$, $S^{(1)}S^{(2)}S^{(3)}S^{(4)}$, etc.

3. Probability rules under knowledge known to be pure

3.1 Complete sample spaces and basic sets of propositions

Some sample spaces qualify as being ‘complete’. The propositions of a complete sample space S are all the propositions referring to a qualifying set* of intrinsic dynamical properties of some quantum mechanical system S during a specified period of time (e.g. from t_0 to t_1 inclusive).† Each atomistic proposition of a complete sample space S is a claim of an entire history of the nominated dynamical properties of S over the time period covered by S . Any less specific claim about the nominated dynamical properties of S can clearly be expressed as a disjunction of these atomistic propositions.

Out of all the propositions of a complete sample space S there are ‘basic sets’ (denoted x, y, \dots) of mutually exclusive and exhaustive propositions. These special sets are of fundamental importance with regard to pure states of knowledge.‡

The members of a basic set of propositions of S (also called a ‘basis’ or ‘propositional basis’ in S) are propositions claiming that one or other of the allowed values of a dynamical property P of S applies at one particular time. They will be distinguished by the value of a single parameter (e.g. by i). So x_i, y_j, \dots will denote the propositions in the bases x, y, \dots respectively generally referring to different times. The basic general dynamical property to which a basis y refers will be denoted by P_y and the

* Which sets qualify for the purpose of forming a complete sample space will be known from our general knowledge G .

† By a ‘quantum mechanical system S ’ we may sometimes mean a part or separate aspect of a (larger) quantum mechanical system. With regard to a single (quantum mechanical) particle, all propositions about certain dynamical properties of the orbital motion of the particle from time t_0 to t_1 , e.g. all propositions about its position (or about its position and momentum) during that time period (but not, say, about its distance from another quantum mechanical particle, which distance is not an *intrinsic* property) constitute a complete sample space. So do all propositions about certain dynamical properties of the spinning motion of the particle from time t_0 to t_1 (e.g. all propositions about the (discrete) z components of spin relative to any number of fixed coordinate systems). The orbital and spinning motions of the particle are ‘separate aspects’ of its total intrinsic dynamics.

‡ Whether or not particular knowledge is pure will be known from our general knowledge.

particular (quantified) dynamical property to which y_j refers will be denoted by P_{y_j} . We will say dynamical property P_y serves as a basis in S . We may think of i and j etc as integer parameters in the range $1,2,\dots,N$ so the sets of propositions x_i, y_j etc are sets with an equal number N of members. We call N the ‘order’ of S and it is generally dependent on the nature of the quantum mechanical system S . In the end however, we may have to allow N to tend to infinity so that i and j etc can range over a finite or countably infinite set of real numbers, or become real continuously variable parameters*. They may actually have to stand for a *number* of real parameters used to enumerate the members of the basis. Being mutually exclusive and exhaustive, just one of the N propositions x_i of a basis x must be actually true while the others are all false. Consequently any basis represents a partitioning of S .†

Let $S^{(1)}$ and $S^{(2)}$ be two complete sample spaces of propositions referring to different systems $S^{(1)}$ and $S^{(2)}$ from time t_0 to time t_1 or to separate aspects $S^{(1)}$ and $S^{(2)}$ of the same system from time t_0 to time t_1 . They are necessarily separate sample spaces (i.e. they have no propositions in common) because systems $S^{(1)}$ and $S^{(2)}$ have no intrinsic dynamical properties in common. Then the sample space combination $S^{(1)}S^{(2)}$ referring to the combined system $S^{(1)}S^{(2)}$ is always complete. And provided the systems contain no indistinguishable identical particles the following rule regarding bases holds true:

Rule for combining bases If the propositions $x_i^{(1)}$ $i = 1,\dots,N$ (referring to time t) form a basis in $S^{(1)}$ and the propositions $x_j^{(2)}$ $j = 1,\dots,M$ (referring to the same time t) form a basis in $S^{(2)}$ then the

* The case of an infinite countable set of integers or of continuous variation should, as we have said, be regarded as a limiting case as the number N of propositions tends to infinity. When taking this limit, the domain of a continuous parameter should be divided into parts of equal natural measure (as in ordinary probability theory), then the principle of indifference (section 5.2) and the principle of maximum entropy (section 7) can be applied unambiguously.

† In applications, sets of propositions that constitute bases will have to be declared as part of our general knowledge. For example, in the complete sample space relating to the position and momentum of a single particle in the time period t_0 to t_1 we have a basis x with propositions x_i where i stands for a volume element $(d^3\mathbf{r})_i$ - one of an infinite number of equal volume elements filling all space - with x_i claiming the particle occupies $(d^3\mathbf{r})_i$ at time t (where $t_0 \leq t \leq t_1$). We also have a basis y with propositions y_j where j stands for a volume element $(d^3\mathbf{p})_j$ - one of an infinite number of equal elements filling all momentum space - with y_j claiming the tip of the particle momentum vector occupies $(d^3\mathbf{p})_j$ at time t . Bases referring to the same dynamical property at different times (we call these ‘time-dependent bases’) will be distinguished by treating them as functions of time; for example the basis x_i claiming a particle occupies one or other of the volume elements $(d^3\mathbf{r})_i$ at a specified time t may be written as $x_i(t)$ to make explicit (and to generalise) the time to which x_i refers.

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set of conjunctions $x_i^{(1)} x_j^{(2)}$ $i = 1, \dots, N$ $j = 1, \dots, M$ form a basis in $S^{(1)}S^{(2)}$ referring to time t . And the number of propositions of this basis, and therefore the order of $S^{(1)}S^{(2)}$, is NM .

This generalises naturally to the case of any number of contemporary, complete and separate sample spaces. So for example if $S^{(3)}$ is a third complete sample space referring to $S^{(3)}$ (distinct from $S^{(1)}$ and $S^{(2)}$) and contemporary with $S^{(1)}$ and $S^{(2)}$, and $x_k^{(3)}$ $k = 1, \dots, L$ is a basis in $S^{(3)}$ (referring to time t), then $S^{(1)}S^{(2)}S^{(3)}$ is a complete sample space (order NML) and the $x_i^{(1)} x_j^{(2)} x_k^{(3)}$ (for all i, j and k) form a basis in $S^{(1)}S^{(2)}S^{(3)}$.*

3.2 Closed sample spaces, pure states of knowledge and the uncertainty principle

Sample spaces can be ‘closed’. Such sample spaces are always separate from one another and complete and in addition they are causally and cognitively independent of one another.† If they cover the same time period they are ‘contemporary’ otherwise they are ‘non-contemporary’. The parts of a system S to which a closed sample space S refers are generally not in interaction with and are clearly distinguishable from the parts of any other system during the time period covered by S .‡ Whenever we say a sample space S is closed we will imply it is a complete sample space, and whenever we say we have pure knowledge with regard to (or in relation to) a sample space S we will imply that S is closed and we have pure knowledge of the system S over the time period covered by S . As we explain soon, any state of pure knowledge is expressible as a probability distribution over certain propositions of a closed sample space.

If $S^{(1)}, S^{(2)}, \dots$ are closed contemporary sample spaces referring to distinct systems $S^{(1)}, S^{(2)}, \dots$ their combination $S = S^{(1)}S^{(2)} \dots$ is always a closed sample space referring of course to the combined system $S = S^{(1)}S^{(2)} \dots$.

Now whenever knowledge Y in relation to a closed sample space S is pure, it is based on measurements conducted before the time period to which S relates. Under pure knowledge Y the propositions of any basis in S have calculable probabilities with determinate relative phases. For example, the x_i of a basis x in S have calculable probabilities $\Phi(x_i|Y)$ $i = 1, \dots, N$ with determinate relative phases. In relation to S , and on

* We stress that this rule for constructing bases in a combination of complete sample spaces safely holds only when, as we have said, the component systems and their combinations do not contain identical particles. The question of bases in the case of systems containing identical particles will be considered separately in Chapter X.

† Which separate and complete sample spaces are *closed* will be known from our general knowledge. Causal and cognitive independence are of course not necessarily present if the sample spaces are merely separate and complete.

‡ As an example, S is closed when the propositions of S refer to the motion between times t_0 and t_1 of a single particle that (between those times) occupies its own region of space far away from other particles and is therefore distinguishable from all other particles and not in interaction with them.

account of the uncertainty principle no significant knowledge in addition to knowledge Y can possibly be held before the time period covered by S . So in relation to S , previous knowledge becomes redundant. We refer here to previous knowledge bearing upon dynamical properties of the system S before the measurements that led to knowledge Y were conducted.* But it is also true that, in relation to S , any *general* knowledge concerning the properties of the system S at times *before* the time period covered by S becomes redundant.†

If in addition to pure knowledge Y we hold knowledge about the state of the system S acquired *after* the period covered by S ,‡ our knowledge in relation to S ceases to be pure and the probabilities over most bases in S seemingly become indeterminate or at least have indeterminate relative phases.

We suppose there is, in principle, the possibility of acquiring at the beginning of, or before the time period covered by S , knowledge of the truth of any one proposition y_j of any basis y in S .§ When so acquired, knowledge y_j of basis y always constitutes pure knowledge in relation to S .

Except in special cases, we cannot acquire, at the beginning of or before the time period covered by S , knowledge of the truth of the conjunction $x_i y_j$ of two propositions x_i , y_j from different bases x and y in S .** And accordingly (except in the special

* At most, such previous knowledge when included in Y can affect only the unimportant absolute phase of the probability distribution $\Phi(x_i|Y)$ $i = 1, \dots, N$.

† E.g. the formula for the potential energy of the particles of the system at times *before* the time period covered by S

‡ This is possible if, at the end of the time period covered by S , we measure a quantity that we know has remained constant (though previously unknown) during the time period covered by S . See section 2.3 of Chapter XV.

§ This assumption is needed in order that transformation functions $\Phi(x_i|y_j)$ (introduced in section 3.4) have meaning and exist for any basis y of S and for any value of the suffix j . So if S covers times t_0 to t_1 and y refers to time t ($t_0 < t < t_1$) we assume it is possible to know the value y_j of y that occurs at time t even before time t_0 . For example, to know y_j might mean that we know (at or before time t_0) the position a particle will have at time t . By Schrödinger's equation, this amounts to knowing the particle wave function (over position at time t_0) that leads to a delta wave function at time t . So if we assume (as we do) that pure knowledge at time t_0 represented by any wave function is essentially a possibility, the possibility of knowing the truth of y_j at time t is also granted. Under knowledge that particle potential is infinite in some regions of space a law applies that states that the particle may not occupy any volume element of space in those regions and in that case we cannot learn the truth of y_j if this proposition claims such a location for the particle. In such cases a limiting approach to the value of the potential has to be taken at any stage of which the truth of any of the y_j could in principle be known.

** Special cases arise when x and y are 'equivalent' bases (see section 3.10), then (for particular values of i and j) y_j implies x_i and vice versa. Then we *could* know the truth of $x_i y_j$ and there is more than one way we could. We might acquire knowledge of y_j by system preparation and then we automatically

cases) the *probabilities* of conjunctions $x_i y_j$ do not exist. Therefore there are generally no pure state joint probability distributions of the kind $\Phi(x_i y_j | Y)$ ($i = 1, \dots, N, j = 1, \dots, N$). The same limitations apply to three or more propositions x_i, y_j, z_k, \dots drawn from three or more different bases x, y, z, \dots in S . Therefore under pure knowledge in a complete sample space by no means all the propositions of the sample space have probabilities.*

On account of the second of (2.3.3) we have, for any basis y , the normalisation rule

$$\sum_{j=1}^N |\Phi(y_j | Y)|^2 = 1. \quad (3.2.1)$$

This must of course hold whether knowledge Y is pure or not.

3.3 Representation of pure states

When knowledge Y in relation to S is pure, we can, as we have said, always derive by logical argument based on the physical laws of quantum mechanics and (complex-valued)

have knowledge of x_i (and therefore of $x_i y_j$) or we might acquire knowledge of x_i by preparation and then we automatically have knowledge of y_j (and therefore of $x_i y_j$). (The methods used in acquiring knowledge of y_j or of x_i are physically different, and might leave the part of the world under investigation in different physical conditions.) In general, x_i and y_j claim incompatible properties and, we can in no way learn the truth of $x_i y_j$ beforehand. For having acquired knowledge of say y_j beforehand we would need to acquire knowledge of x_i beforehand and, by the uncertainty principle, we would then no longer be sure of the truth of y_j . (In a special case of another kind (where x_i and y_j claim incompatible properties), we could learn the truth of $x_i y_j$ in relation to S if for example x_i referred to time t_0 and y_j to time t_1 (t_0 and t_1 being the earliest and latest times in the time period covered by S), and y_j was a primary basis representing a property demonstratively constant during the time period covered by S . This does not however give rise to a pure state of knowledge in S and it requires acquisition of knowledge (of y_j) at time t_1 , i.e. at the end of the time period covered by S as well as acquisition of knowledge (of x_i) at the beginning.)

* These restrictions on existent probabilities are only claimed under conditions of the perfect accuracy associated with pure states. If approximations are allowed things are more open. We know for example that in the classical limit of quantum mechanics properties like the position and momentum of a particle are simultaneously knowable (to classical accuracy) and joint probability distributions over them are sometimes determinate in the classical context (see end of section 10 of Chapter XIV). Under pure knowledge though, the only existent probabilities are those of the propositions belonging to any basis (including any improper or pseudo basis to be defined later) and the disjunctions of the propositions belonging to any one basis. Of course, a proposition that is equivalent to any one of these also has a probability under pure knowledge.

probability theory, a probability distribution over the propositions of any basis of S . This distribution always has determinate relative phases and sometimes even has determinate absolute phases. If we choose a basis y , the probability distribution going with the pure knowledge in relation to S , i.e. $\Phi(y_i|Y)$, is said to express that knowledge ‘in the y representation’ or to be ‘our wave function in the y representation’. If we choose another basis x , we have an alternative probability distribution (or wave function) $\Phi(x_i|Y)$ representing the same pure state of knowledge. This provides a *complementary* representation of our knowledge Y .

To assist us in the derivation of wave functions from pure states of knowledge we claim that wave functions may not be just *any* distributions with determinate relative or absolute phases. There are generally restrictions imposed on them by physical or logical laws. For example they have *logically* to be single-valued and continuous differentiable functions of any continuous variables specifying the propositions of the basis in question* and they may have to be functions that vanish for some values of those variables because some *physical* law renders these particular propositions false.† Also wave functions must logically be continuous differentiable functions of any continuous *parameters* that may be needed to quantify the pure state of knowledge in question.‡

A wave function can therefore only be an *allowed* probability distribution in the sense that all these physical or logical requirements must be satisfied by it.

If, with respect to any basis x , two or more states of knowledge Y, Y', \dots result in wave functions $\Phi(x_i|Y), \Phi(x_i|Y'), \dots$ the same except for constant phase factors, those states of knowledge amount to one and the same pure state of knowledge of the dynamical properties of the system. To within a constant phase factor, there is a 1-1 correspondence between wave functions and pure states of knowledge of a system’s dynamics. And any allowed wave function for a system can be reached, *at least to within a constant phase factor*, by the acquisition of an appropriate pure state of knowledge.§

3.4 Transformation functions between bases

Let x_i and y_j be the general propositions of bases x and y of a complete sample space S of order N . Then there is always the possibility that we know y_j is true. There is therefore a calculable set of wave functions $\Phi(x_i|y_j)$ which we call ‘transformation functions’ or more specifically ‘transformation functions from y to x ’ associated with these bases. These transformation functions are calculable at least to within an

* An exception (to continuity) arises in the case of wave functions over a proper basis for a system of identical fermions (see section 6.1 of Chapter X).

† For example, as we have said before, a particle may not occupy a region of infinite potential, so the wave function over position must vanish in such a region.

‡ This law is used in section 8.1 in connection with the extension of the similarity principle. Unless otherwise stated, wave functions are always assumed to be normalised as in (3.2.1).

§ An explicit example of the generality of wave functions and pure states of knowledge is given in section 6 of Chapter VII.

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indeterminate constant phase factor $e^{i\alpha}$ independent of i and j .^{*} In the calculation of transformation functions use can be made of the following general laws of probability (as well as the principles of probability assignments in section 5).

Law of reciprocity of transformation functions

Transformation functions are related reciprocally, i.e. (with the star denoting the complex conjugate)

$$\Phi(y_j|x_i) = (\Phi(x_i|y_j))^* \quad (3.4.1)$$

for all i and j .

Law of unit determinant (in case the bases are discrete and of finite dimension)

If the bases, i.e. the labels i and j , are discrete, finite in number, and have a natural order, the determinate of $\Phi(x_i|y_j)$ regarded as a square matrix $[\Phi(x_i|y_j)]$ is equal to 1, i.e.

$$\det[\Phi(x_i|y_j)] = 1 \quad (3.4.2)$$

the matrix being defined so the order of the rows from top to bottom coincides with the natural order of the i values and the order of the columns from left to right coincides with the natural order of the j values.

We will refer to (3.4.2) as ‘Feynman phase normalisation’ (see p.6-5 of [7]).

Law of orthonormality of transformation functions

Viewed as probability distributions over the variable i for the various values of j , transformation functions $\Phi(x_i|y_j)$ are, always orthonormal, i.e. always both normalised and mutually orthogonal[†]:

^{*} If the $\Phi(x_i|y_j)$ contained a phase factor $e^{i\alpha_j}$ indeterminate and *different* for each value of j , then a wave function $\Phi(x_i|Y)$ derived using Feynman’s law (3.5.1) would have indeterminate relative *moduli* for different i contrary to the rules of quantum mechanics. (We will see in fact that many transformation functions $\Phi(x_i|y_j)$ have *fully determinate* phases.)

[†] Therefore when i and j are discrete and finite in number (3.4.1) and (3.4.3) alone imply

$\det[\Phi(y_k|x_i)]\det[\Phi(x_i|y_j)] = |\det[\Phi(x_i|y_j)]|^2 = \det[\delta_{ij}] = 1$ or $\det[\Phi(x_i|y_j)] = e^{i\beta}$, where $0 \leq \beta < 2\pi$, and this shows the possibility of Feynman phase normalisation by division of all (pre-phase-normalised) elements $\Phi(x_i|y_j)$ by $e^{i\beta/N}$ where N is the number of i (or j) values i.e. the order of the

$$\sum_{i=1}^N (\Phi(x_i|y_k))^* \Phi(x_i|y_j) = \delta_{kj}. \quad (3.4.3)$$

Law of completeness of transformation functions

Any set of transformation functions $\Phi(x_i|y_j)$ are ‘complete’ in the sense that any wave function $\Phi(x_i|Y)$ (i.e. any probability distribution over the basis x under pure knowledge Y) can be expressed as a linear combination of the $\Phi(x_i|y_j)$:

$$\Phi(x_i|Y) = \sum_{j=1}^N a_j \Phi(x_i|y_j) \quad (3.4.4)$$

where the a_j are complex constants.

Sum rule for transformation functions

The general sum rule (in section 2.3) applies of course to any transformation function $\Phi(x_i|y_j)$ viewed as a probability distribution over the propositions of the basis x_i . Since the propositions of any basis are mutually exclusive we have, by (2.3.2), that the probability of a disjunction, e.g. $x_4 + x_7 + \dots$, of any set of the basic propositions, m in number, is given by

$$\Phi(x_4 + x_7 + \dots|y_j) = e^{i(\eta_j - k_j)} \sqrt{|\Phi(x_4|y_j)|^2 + |\Phi(x_7|y_j)|^2 + \dots} \quad (3.4.5)$$

where k_j is the phase characteristic of knowledge y_j and η_j the phase characteristic of the disjunction $x_4 + x_7 + \dots$ under knowledge y_j .

If, however, the individual phases characteristic of the members of the disjunction under knowledge y_j have the same value λ_j , e.g. if

$$\text{ch}(x_4|y_j) = \text{ch}(x_7|y_j) = \dots = \lambda_j \quad (3.4.6)$$

and the members of disjunction do not include all propositions of the basis, then in (3.4.5) we claim

$$\eta_j = \lambda_j. \quad (3.4.7)$$

sample space. But, as we have said, we suppose this normalisation *necessarily* applies whenever the labels i (and j) have a natural order.

If, in addition, our degrees of belief in the members of the disjunction are equal, so that their probabilities are equal:

$$\Phi(x_4|y_j) = \Phi(x_7|y_j) = \dots \quad (3.4.8)$$

then the probability of the disjunction under knowledge y_j is accordingly equal to \sqrt{m} times that of any one of the basic propositions making up the disjunction, so for example

$$\Phi(x_4 + x_7 + \dots | y_j) = \sqrt{m} \Phi(x_4 | y_j). \quad (3.4.9)$$

3.5 Feynman's law

We can now formulate the relation between wave functions representing the same pure state of knowledge.*

Feynman's Law

Any two representations of a pure state of knowledge by probability distributions $\Phi(x_i|Y)$ and $\Phi(y_j|Y)$ using bases x and y in S are related thus:

$$\Phi(x_i|Y) = \sum_{j=1}^N \Phi(x_i|y_j) \Phi(y_j|Y). \quad (3.5.1)$$

More generally, if Z is any proposition claiming a particular dynamical property of the system S to which S relates such that knowledge Z would constitute pure knowledge of S , then for any basis y_j in S

$$\Phi(Z|Y) = \sum_{j=1}^N \Phi(Z|y_j) \Phi(y_j|Y). \quad (3.5.2)$$

The existence of indeterminate constant phase factors in some wave functions means we can *to a limited extent* multiply those wave functions by constant phase factors without changing the relations between them that the (complex-valued) probability calculus requires. For example if transformation functions $\Phi(x_i|y_j)$ have only determinate *relative* phases we can multiply them all by $e^{i\alpha}$ where α is a real numerical

* We call this relation 'Feynman's law' because it was first interpreted by Feynman as a law of probabilities (see p.6-1 of [7] and p.111 of [16]).

constant independent of i and j . But then we must multiply all the $\Phi(y_j|x_i)$ by $e^{-i\alpha}$ because of the reciprocity relation (3.4.1). And if the transformation functions are discrete and finite in number the requirement (3.4.2) means α must satisfy $N\alpha = 2\pi m$ where N is the order of the sample space (or of the determinant) and m any positive or negative integer or zero.

Also (3.5.1) relates any indeterminate constant phase factors that may be present in wave functions $\Phi(x_i|y_j)$, $\Phi(x_i|Y)$ and $\Phi(y_j|Y)$. So if for example only the $\Phi(x_i|y_j)$ have determinate absolute phases and we multiply the wave function $\Phi(y_j|Y)$ in one representation by a constant phase factor we should multiply the wave function $\Phi(x_i|Y)$ in the other representation by the *same* phase factor.

When fixing phases of wave functions (whose phases are not absolutely determinate) in a *conventional* way, we must be constantly aware of required relations that reduce the number of *independent* indeterminate phases otherwise contradictions will of course arise.

Note that, although (3.5.1) resembles the classical relation between distributions, it cannot be derived from the sum and product rules of section 2. Relation (3.5.1) (or more generally (3.5.2)) stands alone as the only source of the ‘interference of probabilities’ characteristic of quantum theory. The present theory of complex-valued probability differs from others in that the ‘interference of probabilities’ does not arise as a result of the sum rule. That is, we do not claim $\Phi(A+B|Y) = \Phi(A|Y) + \Phi(B|Y)$ in place of (2.3.1) or claim that the product rule (2.4.1) or something like it holds when A and B claim incompatible properties, as would be needed to *derive* (3.5.1). Such claims lead to contradictions or to violations of necessary properties of probability.*

Feynman’s law is the general quantitative expression of the uncertainty principle in the new probability calculus. In the form (3.5.1) it determines the way and the extent to which, under changing pure knowledge Y , one probability distribution becomes broader while another becomes narrower.

3.6 Primary bases and the possibility of harmless conditioning

Certain bases of a complete sample space S may be ‘primary’.[†] With regard to these we maintain the following properties.

* E.g. if $\Phi(A+B|Y) = \Phi(A|Y) + \Phi(B|Y)$ holds in place of (2.3.1), the probability of a disjunction of mutually exclusive propositions A and B can be zero while, under the same knowledge, the probabilities of A and B , i.e. $\Phi(A|Y)$ and $\Phi(B|Y)$ are non-zero. This is difficult to reconcile with the idea that probability measures degree of belief.

[†] Which are primary will be known from our general knowledge. For example, in a sample space relating to all properties of the orbital motion of a particle, the propositions claiming the particle occupies one or other volume element of space at a particular time constitute a primary basis, but the propositions claiming the particle momentum occupies one or other volume element of momentum space at a particular time probably do not because an instantaneous and precise measurement of the momentum seems certain to change it by a very large amount (see for example p.152 of [12]).

Having obtained knowledge Y of a system S pure in relation to a representative sample space S covering a time period t_0 to t_1 , we claim (as part of our general knowledge G) that we can, by observation, learn by chance at time t_2 (where $t_0 < t_2 < t_1$) the truth of the disjunction of any number of the propositions x_i of any primary basis x of S referring to time t_2 .^{*} This can, we claim, be accomplished instantly and harmlessly with respect to proposition Y [†] and the propositions x_i of basis x (but not in general harmlessly with respect to other bases of S). Let A be the proposition representing the disjunction.

From time t_2 we then have pure knowledge AY in relation to a sample space S' which includes only those propositions of S that relate to times from t_2 to t_1 . The bases of S' (which include the basis x) are a subset of the bases of S . We call the process of passing from knowledge Y pure in relation to sample space S to knowledge AY pure in relation to sample space S' , 'harmless conditioning'.

So after harmless conditioning, the sample space in which our pure knowledge is expressed remains complete and closed but shrinks to one covering a shorter time period.

An extreme case of harmless conditioning occurs when, by observation, we learn by chance at time t_2 the truth of one of the propositions, say x_i , of a primary basis x of S referring to time t_2 . This we suppose is a possibility so long as x_i does not have probability zero under knowledge Y . And as in the case of learning by chance the truth of a disjunction of the propositions x_i , our sample space then contracts from S to S' .

3.7 The product rule for wave functions and the law of absolute logical independence under pure knowledge

We first give rules concerning bases and wave functions in a combination of closed sample spaces referring to distinct systems (or distinct aspects of a single system). Then we state the law of absolute logical independence under pure knowledge. Because the sample spaces are closed, all we say is true whether or not the systems in question or their combinations include identical particles.

Rule for combining bases of closed sample spaces

Let $x_i^{(1)}$ be a basis pertaining to time t in a closed sample space $S^{(1)}$ and let $x_j^{(2)}$ be a basis pertaining to the same time t in another closed sample space $S^{(2)}$ covering the same time period. Then the set of conjunctions $x_i^{(1)}x_j^{(2)}$ labelled by

^{*} We omit disjunctions which have probability zero under knowledge Y .

[†] Note that it may be necessary to replace Y by an equivalent proposition in order to ensure the possibility of this. This would be necessary if, for example, Y claimed a basic property y_j referring to a time after t_2 ; then Y would have to be replaced by an equivalent proposition claiming a property of S occurring at or before time t_2 .

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(i, j) always constitute a basis pertaining to time t in $S^{(1)}S^{(2)}$. If bases $x_i^{(1)}$ and $x_j^{(2)}$ are primary then so is basis $x_i^{(1)}x_j^{(2)}$. But whether or not the bases are primary the following rule also applies.

Product rule for wave functions

If we hold pure knowledge $Y^{(1)}$ in relation to $S^{(1)}$ and simultaneously hold pure knowledge $Y^{(2)}$ in relation to $S^{(2)}$, then knowledge $Y^{(1)}Y^{(2)}$ in relation to $S^{(1)}S^{(2)}$ is pure and our wave function in the $x_i^{(1)}x_j^{(2)}$ representation in $S^{(1)}S^{(2)}$ is the product of our wave functions in the $x_i^{(1)}$ representation and the $x_j^{(2)}$ representation in $S^{(1)}$ and $S^{(2)}$ respectively, i.e.

$$\Phi(x_i^{(1)}x_j^{(2)}|Y^{(1)}Y^{(2)}) = \Phi(x_i^{(1)}|Y^{(1)})\Phi(x_j^{(2)}|Y^{(2)}). \quad (3.7.1)$$

Conversely if our wave function under pure knowledge Y in relation to $S^{(1)}S^{(2)}$ using the basis $x_i^{(1)}x_j^{(2)}$ in $S^{(1)}S^{(2)}$, resolves into normalised factors f_i and g_j so that

$$\Phi(x_i^{(1)}x_j^{(2)}|Y) = f_i g_j$$

and $S^{(1)}$ and $S^{(2)}$ are separately closed, then our knowledge Y must be separable into knowledge $Y^{(1)}$ pure in relation to $S^{(1)}$ and knowledge $Y^{(2)}$ pure in relation to $S^{(2)}$ * (i.e. $Y = Y^{(1)}Y^{(2)}$) and we should put, for our wave functions in the $x^{(1)}$ and $x^{(2)}$ representations,

$$\Phi(x_i^{(1)}|Y^{(1)}) = f_i e^{i\alpha} \quad \text{and} \quad \Phi(x_j^{(2)}|Y^{(2)}) = g_j e^{-i\alpha} \quad (3.7.2)$$

where α is generally an indeterminate real constant.†

* Knowledge Y pure in relation to $S^{(1)}S^{(2)}$ is not of course *necessarily* separable into pure knowledge in relation to $S^{(1)}$ and pure knowledge in relation to $S^{(2)}$. It generally is not, for example, if after acquiring knowledge Y systems $S^{(1)}$ and $S^{(2)}$ interact before the time period covered by $S^{(1)}$ and $S^{(2)}$.

† Sometimes a wave function $\Phi(x_i^{(1)}x_j^{(2)}|Y)$ in a closed product space $S^{(1)}S^{(2)}$ factors but $S^{(1)}$ and $S^{(2)}$, though *complete* sample spaces, are not (separately) *closed*. An example of this kind of factoring occurs in the case of spinning and orbital motion of a spin one-half particle in an x dependent magnetic field with only a z component under pure knowledge that includes knowledge of the z component of spin; the Schrödinger equation is then of the form (3.1.3) of Chapter XIII which has factored solutions like $\delta_{\sigma,1/2}g(\mathbf{r},t)$ yet the sample spaces S_σ and S_r for the spin and orbital motions of the particle are not separately closed because the spin and orbital aspects of motion are not generally independent.

The rule for combining bases of closed sample spaces and the product rule for wave functions (together with its converse) generalise to cases of any number of contemporary and closed sample spaces.* And the sample spaces need not be of the same order.

We now state the law of absolute logical independence under pure knowledge.

Law of absolute logical independence under pure knowledge

Suppose we hold pure knowledge $Y^{(1)}$ in relation to $S^{(1)}$ and pure knowledge $Y^{(2)}$ in relation to another (closed but not necessarily contemporary) sample space $S^{(2)}$. Then $S^{(1)}$ and $S^{(2)}$ are *necessarily* logically independent sample spaces under knowledge $Y^{(1)}Y^{(2)}$.

This law generalises to the case of pure states of knowledge $Y^{(1)}, \dots, Y^{(n)}$ held in relation to any number of closed but not necessarily contemporary sample spaces $S^{(1)}, \dots, S^{(n)}$. Since our knowledge with regard to each sample space is pure those sample spaces are necessarily logically independent of one another under knowledge $Y^{(1)} \dots Y^{(n)}$.

3.8 The observational equivalence of wave functions differing only in absolute phase

Suppose two wave functions $\Phi(x_i|Y)$ and $\Phi(x_i|Y')$ over a basis x_i of a sample space S relating to a system S (a part of the physical world) differ only by a constant phase factor, i.e.

$$\Phi(x_i|Y) = \Phi(x_i|Y')e^{i\alpha} \tag{3.8.1}$$

where α is a constant phase independent of i . Then, by Feynman's law (3.5.1), the same simple relation will hold between the wave functions in any other representation, i.e. relation (3.8.1) is independent of the basis x , or α is the same in every basis. In general Y and Y' will claim different properties of the physical world (for example different properties of S or different properties of preparation apparatus applied to S) but the

* The converse of the generalised product rule for wave functions is demonstrated by grouping the propositions of the bases. For example, in the case of three contemporary and closed sample spaces $S^{(1)}$, $S^{(2)}$ and $S^{(3)}$ with bases $x^{(1)}$, $x^{(2)}$ and $x^{(3)}$ respectively, all pertaining to the same time t , if $\Phi(x_i^{(1)} x_j^{(2)} x_k^{(3)}|Y) = f_i g_j h_k$ then $\Phi((x_i^{(1)} x_j^{(2)}) x_k^{(3)}|Y) = (f_i g_j) h_k$ and the rule for just two sample spaces gives $\Phi(x_i^{(1)} x_j^{(2)} x_k^{(3)}|Y) = \Phi(x_i^{(1)} x_j^{(2)}|Y) \Phi(x_k^{(3)}|Y)$ where $\Phi(x_i^{(1)} x_j^{(2)}|Y) = f_i g_j e^{i\alpha}$, and $\Phi(x_k^{(3)}|Y) = h_k e^{-i\alpha}$. This in turn becomes $\Phi(x_i^{(1)} x_j^{(2)} x_k^{(3)}|Y) = \Phi(x_i^{(1)}|Y) \Phi(x_j^{(2)}|Y) \Phi(x_k^{(3)}|Y)$ where $\Phi(x_i^{(1)}|Y) = f_i e^{i\beta}$, $\Phi(x_j^{(2)}|Y) = g_j e^{i\alpha} e^{-i\beta}$ and $\Phi(x_k^{(3)}|Y) = h_k e^{-i\alpha}$.

states of knowledge Y and Y' are always ‘observationally equivalent’ with regard to S in the sense that (on account of relation (3.8.1)) the calculated expected frequencies of the possible outcomes of any measurement conducted on the system S are necessarily the same.* This is a necessary condition for us to be able to claim as we have (in section 3.3) that under (3.8.1) Y and Y' amount to the *same* pure state of knowledge of the dynamical properties of the system S .

3.9 Extension of a sample space

Suppose S is a complete sample space of order N consisting of propositions relating to certain dynamical properties of a system S over a given time period. Then there may be other dynamical properties of S that are known to us but not mentioned in any of the propositions of the closed sample space S .†

There is no reason why one or more of such other dynamical properties should not be incorporated into S . That is, we may if we wish extend S to include all propositions relating to dynamical properties of S already referred to in S *and* all propositions relating to one or more other properties (or to both one or more of the original properties *and* one or more of the other properties). The resulting sample space is still a *complete* sample space of order N .

Unless otherwise stated it will be supposed that any closed sample space S of order N is fully extended to include all propositions about any real dynamical properties of the system S over the given time period.

3.10 Equivalent bases

The theory of equivalent bases is developed in section 10.1 of Chapter II. Here we give a limited account of that theory for the purpose of formulating the law of inferred dynamical properties in section 3.12.

In a sample space S of order N relating to a system S it can be that (with appropriate ordering of the propositions of bases) respective propositions of two or more bases $y_j, y'_j \dots$ etc. ($j = 1, \dots, N$), while claiming distinct physical properties, nonetheless *imply* one another (on account of physical correlation of the properties concerned). They may imply one another with known phases of implication, so for example $y'_j^{-\alpha_j} \Leftrightarrow^{\alpha_j} y_j$ where the α_j are known. The transfer functions between these bases are then diagonal, e.g.

* See the calculation of expected frequencies in section 9 of Chapter II.

† For example, there may be inferred dynamical properties associated with complete sets of orthogonal wave functions (see section 3.12) that may not be mentioned by any proposition of S .

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$$\Phi(y_i|y'_j) = \delta_{ij} e^{i\alpha_j}$$

$$\Phi(y_i|y''_j) = \delta_{ij} e^{i\beta_j}$$

...

where α_j, β_j, \dots are all known phases for $j=1, \dots, N$, and we say that y_j, y'_j, \dots are 'equivalent bases correspondingly ordered'. (They need not necessarily be bases referring to the same time.) Then the wave functions over a basis x_i (not equivalent to the bases y_j, y'_j, \dots etc.) under the pure states of knowledge y_j, y'_j, \dots are the same to within constant phase factors. This is because, by Feynman's law

$$\Phi(x_i|y'_j) = \sum_l \Phi(x_i|y_l) \Phi(y_l|y'_j) = \sum_l \Phi(x_i|y_l) \delta_{lj} e^{i\alpha_j} = \Phi(x_i|y_j) e^{i\alpha_j}$$

and similarly

$$\Phi(x_i|y''_j) = \Phi(x_i|y_j) e^{i\beta_j}$$

and so on. So $\Phi(x_i|y_j), \Phi(x_i|y'_j), \Phi(x_i|y''_j), \dots$ are the same to within a constant phase factor when y_j, y'_j, y''_j, \dots are equivalent bases correspondingly ordered. And y_j, y'_j, y''_j, \dots (for any one value of j) are different propositions concerning system S that serve to represent the same pure state of knowledge of dynamical properties of the system S .

3.11 General law of reciprocity and the extension of the sum rule for transformation functions to wave functions of any kind

General law of reciprocity

Let S be a complete sample space whose propositions concern a system S . If Y and Z are propositions of S claiming dynamical properties of S and if knowledge Y would constitute a pure state of knowledge and if knowledge Z would constitute a pure state of knowledge, then the probability of Y under knowledge Z and the probability of Z under knowledge Y are reciprocally related thus

$$\Phi(Y|Z) = \Phi^*(Z|Y) \tag{3.11.1}$$

the star denoting the complex conjugate.

In the particular case Y and Z are propositions y_j and z_k respectively drawn from bases y and z in S , (3.11.1) becomes the law of reciprocity of transformation functions (already noted in (3.4.1)).

Extension of the sum rule for transformation functions to wave functions of any kind

The general sum rule (in section 2.3) applies of course to any wave function $\Phi(x_i|Y)$ over any basis x_i . And we have, by (2.3.2), that the probability of a disjunction, e.g. $x_4 + x_7 + \dots$ of any set of the basic propositions is given by

$$\Phi(x_4 + x_7 + \dots|Y) = e^{i(\eta-k)} \sqrt{|\Phi(x_4|Y)|^2 + |\Phi(x_7|Y)|^2 + \dots} \quad (3.11.2)$$

where k is the phase characteristic of knowledge Y and η the phase characteristic of the disjunction $x_4 + x_7 + \dots$ under knowledge Y .

If, however, the individual characteristic phases of the members of the disjunction under knowledge Y have the same value λ , e.g. if

$$\text{ch}(x_4|Y) = \text{ch}(x_7|Y) = \dots = \lambda \quad (3.11.3)$$

and the members of the disjunction do not include all propositions of the basis, then in (3.11.2) we claim

$$\eta = \lambda. \quad (3.11.4)$$

And if, in addition

$$\Phi(x_4|Y) = \Phi(x_7|Y) = \dots \quad (3.11.5)$$

then, accordingly

$$\Phi(x_4 + x_7 + \dots|Y) = \sqrt{m}\Phi(x_4|Y), \quad (3.11.6)$$

m being the number of propositions making up the disjunction.

In the particular case that Y is a proposition y_j of a basis y (different from basis x) the above rule clearly becomes the same as the sum rule for transformation functions (noted already in section 3.4).

In section 1 of Chapter X we introduce ‘improper’ bases. We note here that the above extension of the sum rule to wave functions of any kind includes extension to wave functions over improper bases.

3.12 The law of inferred dynamical properties

We now formulate the law of inferred dynamical properties.

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Let S be a closed sample space of propositions relating to the dynamical properties of a quantum mechanical system S over some time period. Let the Y_j ($j=1,\dots,N$) be propositions representing pure states of knowledge in relation to the sample space S of order N . And suppose the corresponding wave functions $\Phi(x_i|Y_j)$ over a basis x in S are orthogonal and form a complete set.* Then we have the following law.

Law of inferred dynamical properties

To the states of knowledge Y_j ($j=1,\dots,N$), regardless of the absolute phases of the wave functions $\Phi(x_i|Y_j)$, there corresponds an ‘inferred’ dynamical property P of S quantified by the variable j , and under knowledge Y_j (for any value of j) P is quantified by j , i.e. quantified property P_j is present during the time period covered by S . Also, to hold knowledge that property P_j is present is to hold a pure state of knowledge.

In the case the wave functions $\Phi(x_i|Y_j)$ are the same (to within constant phase factors) as the transformation functions $\Phi(x_i|y_j)$ or $\Phi(x_i|y'_j),\dots$ from one or other of the correspondingly ordered equivalent bases y, y', \dots to the basis x in S , property P_j (for any one given value of j) is the property that *one or other* of the basic properties $P_{y_j}, P_{y'_j}, \dots$ claimed by y_j, y'_j, \dots is present.†

We note that the law of inferred dynamical properties is different from the other laws of complex-valued probability. All the other laws are claims regarding the values of probabilities or claims regarding the relations between probabilities. They could be described as purely logical laws. But the law of inferred dynamical properties is a claim relating any set of orthogonal probability distributions (wave functions) to a physical property. It forms a bridge between probability theory (i.e. logic) and physics. This can be likened to the situation in general relativity where we have a space-time geometry which can be described mathematically in purely geometric terms but where the claim is made that an aspect of the curvature of space-time is related to a physical property of the

* In the language of ordinary quantum mechanics we would say the wave functions are eigenfunctions of a complete set of commuting Hermitian operators.

† We include the case (if it should arise) where there is a basis y_j which has no equivalent bases. In that case P_j and P_{y_j} are the same property. But generally, although they are physically correlated, the properties $P_j, P_{y_j}, P_{y'_j}, \dots$ are distinct and letting P_j stand for the proposition claiming P_j we note that P_j ($= y_j + y'_j + \dots$) is not the same as any one of the propositions y_j, y'_j, \dots even though (under our general knowledge G) any one of the propositions P_j, y_j, y'_j, \dots implies any other.

matter occupying it. So now concepts in both the logic of science and the geometry of science are associated with properties of matter.

4. Cases of essentially pure knowledge

Sometimes our knowledge Y relating to a closed sample space S of propositions falls short of being pure only because we lack certain knowledge characterised by parameters whose values are unknown but which could in principle be learnt harmlessly with regard to *all* propositions of S . We call such a state of knowledge ‘essentially pure’.

The rules of section 3 specific to *knowledge known to be pure* hold algebraically also in the case of knowledge known to be *essentially pure*. So do the principles of probability assignment in section 5. Using these rules and principles we may be able to establish (from the knowledge we do have) algebraic (or functional) forms for probability distributions over propositions of S . Then when the missing information finally arrives we are able to evaluate fully (i.e. numerically) the pure state probability distributions over propositions of S .

5. Principles of probability assignment

In addition to the calculus of probabilities we have (as in classical Bayesian probability) logical principles of probability assignment that may sometimes be applied to establish the form of prior probability distributions.

The principles of probability assignment are given below. In these, propositions A, B, X, \dots and propositions Y, Z, \dots (representing our knowledge) claim dynamical properties of the physical world and G claims our general knowledge. (In addition to these principles there is the principle of maximum entropy applying under conditions in which complex-valued probability and classical probability coexist (see sections 6 and 7).)*

We start by declaring the uniqueness of degrees of belief or of probabilities under conditions of logical equivalence and we give the ‘general rule for phases’.

First uniqueness principle If (under G) $A \Leftrightarrow B$ and $Y \Leftrightarrow Z$ then $|\Phi(A|Y)|^2 = |\Phi(B|Z)|^2$

Second uniqueness principle If (under G) $A \equiv B$ (i.e. if $A \Rightarrow^0 B$ and $B \Rightarrow^0 A$) and $Y \equiv Z$ (i.e. $Y \Rightarrow^0 Z$ and $Z \Rightarrow^0 Y$) then $\Phi(A|Y) = \Phi(B|Z)$.

General rule for phases If (under G) $A \overset{-\beta}{\Leftrightarrow} B$ (i.e. if $A \Rightarrow^\beta B$ and $B \Rightarrow^{-\beta} A$)

* There are also principles of array assignment in the calculation of probabilities under mixed states of knowledge (see Chapter XIV) and there may of course be other principles of probability assignments yet to be discovered.

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and $Y \stackrel{-\alpha}{\Leftrightarrow} Z$ (i.e. $Y \stackrel{\alpha}{\Rightarrow} Z$ and $Z \stackrel{-\alpha}{\Rightarrow} Y$) then $\Phi(A|Y) = \Phi(B|Z)e^{i(\alpha-\beta)}$.

In words, the first principle states that if (under our general knowledge G) A and B are equivalent and Y and Z are equivalent our *degrees of belief* (in A given Y and in B given Z) are the same. The second principle states that if A and B are *fully* equivalent (which we declare to be the case when for example they claim the same property in different units or in different coordinate systems) and if Y and Z are also *fully* equivalent, our *probabilities* (for A given Y and for B given Z) are the same. The general rule for phases gives the way the phases of the probabilities are generally related under equivalence. We can of course derive the first and second uniqueness principles from the general rule for phases, but for future reference, we write them down explicitly.

5.1 The similarity principle

This takes the following form

Similarity principle

If our knowledge $Y^{(1)}G^{(1)}$ with regard to any one of a (not necessarily mutually exclusive or exhaustive) set of propositions $X_i^{(1)}$ is recognisably *similar** to our knowledge $Y^{(2)}G^{(2)}$ with regard to a respectively labelled and equally numerous set of propositions $X_i^{(2)}$ then for each i we should set

$$\Phi(X_i^{(1)}|Y^{(1)}G^{(1)}) = \Phi(X_i^{(2)}|Y^{(2)}G^{(2)})e^{i\alpha} \quad (5.1.1)$$

where α is some real constant (independent of i).

And more generally, if the problem of finding the probabilities of the $X_i^{(1)}$ under *various* states of knowledge $Y_j^{(1)}G_j^{(1)}$ is recognisably *similar* to the problem of finding the probabilities of the $X_i^{(2)}$ under a respectively labelled and equally numerous set of states of knowledge $Y_j^{(2)}G_j^{(2)}$, then for each i and j we should set

$$\Phi(X_i^{(1)}|Y_j^{(1)}G_j^{(1)}) = \Phi(X_i^{(2)}|Y_j^{(2)}G_j^{(2)})e^{i\alpha} \quad (5.1.2)$$

* In formulating this similarity principle we allow for a possible difference in our general knowledge G in cases (1) and (2). For example, there may be a difference in our supposed knowledge of the rest frame and of potentials experienced by the particles of a system as in section 5 of Chapter IV.

where α is some real constant (independent of i and j).*

It will be pretty clear whether or not one problem of finding a set of probabilities is *similar* to another but a case where similarity might at first appear to apply but generally does not is one in which $G_j^{(1)} = G_j^{(2)} = G$, and for each i , $X_i^{(1)}$ and $X_i^{(2)}$ are equivalent (known to imply one another under G), and for each j , $Y_j^{(1)}$ and $Y_j^{(2)}$ are equivalent. Owing to the existence of phases of implication similarity might actually apply in such a case only when the respective propositions imply one another with the same phase of implication (i.e. when $X_i^{(1)} \stackrel{-\beta}{\Leftrightarrow} X_i^{(2)}$ and $Y_j^{(1)} \stackrel{-\gamma}{\Leftrightarrow} Y_j^{(2)}$ where β and γ are phases independent of i and j). Then, by the general rule for phases, (5.1.2) clearly applies with $\alpha = \gamma - \beta$. But of course such equivalence of $X_i^{(1)}$ and $X_i^{(2)}$, and of $Y_j^{(1)}$ and $Y_j^{(2)}$, under a common general knowledge G , is by no means the only way in which similarity might apply.

But in those many other ways it applies, it does so only when the propositions $X_i^{(1)}$ and $X_i^{(2)}$, and the propositions $Y_j^{(1)}$ and $Y_j^{(2)}$, are in each case making claim to *physically similar* properties and not to properties merely correlated with similar properties. For example, if similarity expressed by (5.1.2) applies to propositions $X_i^{(1)}$ and $X_i^{(2)}$ claiming appropriate (physically similar) properties, it will not apply if the $X_i^{(1)}$ are replaced by propositions $\tilde{X}_i^{(1)}$ (claiming inappropriate but correlated properties) related to the $X_i^{(1)}$ by $X_i^{(1)} \stackrel{-\alpha_i}{\Leftrightarrow} \tilde{X}_i^{(1)}$ where the (all determinate) phases of implication α_i vary with i .

Also, when similarity is claimed we will take it for granted that the propositions $X_i^{(1)}, X_i^{(2)}, Y_j^{(1)}$ and $Y_j^{(2)}$ in question are *plainly* expressed.

Similarity under any knowledge of dynamical properties

Let the Y_j include (under variation of j) *all* possible states of knowledge of the dynamical properties of the physical world (including the state Y_0 of no knowledge of the dynamical properties). And let G be our general knowledge which includes of course our

* Here j is a parameter generally quantifying both our knowledge of dynamical properties and our knowledge of unchanging properties of the system in question. Like i it may in practice take discrete or continuous values or represent a set of such parameter values. Most often $G_j^{(1)}$ and $G_j^{(2)}$ will be independent of j (i.e. just $G^{(1)}$ and $G^{(2)}$) and often $G^{(1)}$ and $G^{(2)}$ will be the same (i.e. $G^{(1)} = G^{(2)} = G$). An example of possible j dependence of G occurs in the application of the similarity principle to demonstrate the symmetry properties of improper wave functions (section 2 of Chapter X).

knowledge of the unchanging properties of the physical world. Then it can happen that the problem of finding the probabilities $\Phi(X_i|Y_jG)$ of the X_i under any one of the states of knowledge Y_j is recognisably *similar* to that of finding the probabilities $\Phi(X_i|Y_{j'}G)$ of the X_i under any other one of the same states of knowledge.* In that case the correct mathematical expression of the similarity is that for any j and j'

$$\Phi(X_i|Y_jG)e^{ik_j} = \Phi(X_i|Y_{j'}G)e^{ik_{j'}} \quad (5.1.3)$$

where (for any j) k_j is the phase characteristic of knowledge Y_j . On putting $j' = 0$ so that $Y_{j'}$ becomes the state of no knowledge of dynamical properties, we can rewrite this as

$$\Phi(X_i|Y_jG)e^{ik_j} = \Phi(X_i|Y_0G) = \Phi(X_i|G) \quad (5.1.4)$$

valid for all j . This is because, by (2.2.1.11), $k_{j'} = 0$ when $j' = 0$.

Similarity under no knowledge of dynamic properties

Furthermore suppose G_j (according to the value of j) denotes one or other of a number of different states of our general knowledge, differing only with regard to our knowledge of the unchanging properties of the physical world. Then if, for any value of j , the problem of finding the probabilities $\Phi(X_i|Y_0G_j)$ of a set of propositions X_i about the physical world is recognisably *similar* to that of finding the probabilities $\Phi(X_i|Y_0G_{j'})$ of the same propositions for any other value j' of j we should set $\Phi(X_i|Y_0G_j)$ equal to $\Phi(X_i|Y_0G_{j'})$ or

$$\Phi(X_i|G_j) = \Phi(X_i|G_{j'}) \quad (5.1.5)$$

for all j and j' .†

Similarity under a change in general knowledge alone

If in (5.1.1) $X_i^{(1)} = X_i^{(2)} = X_i$ (or if $X_i^{(1)}$ and $X_i^{(2)}$ are fully equivalent under general knowledge $G^{(1)}$ and under general knowledge $G^{(2)}$ and X_i stands for either), and if $Y^{(1)} = Y^{(2)} = Y$ (or if $Y^{(1)}$ and $Y^{(2)}$ are fully equivalent under general knowledge $G^{(1)}$

* This kind of similarity occurs in section 6.1 of Chapter X.

† This kind of similarity also occurs in section 6.1 of Chapter X.

and under general knowledge $G^{(2)}$ and Y stands for either), and the problem of finding the probabilities of the $X_i^{(1)}$ under knowledge $Y^{(1)}G^{(1)}$ is recognisably similar to that of finding the probabilities of the $X_i^{(2)}$ under knowledge $Y^{(2)}G^{(2)}$ then we should simply put

$$\Phi(X_i|YG^{(1)}) = \Phi(X_i|YG^{(2)}) \quad (5.1.6)$$

for all i .*

Note that there is no converse to the similarity principle in any of the above forms. So if for example (5.1.2) is true of sets of propositions $X_i^{(1)}$ and $Y_j^{(1)}G_j^{(1)}$, and equally numerable sets of propositions $X_i^{(2)}$ and $Y_j^{(2)}G_j^{(2)}$ with α independent of i and j , it does not necessarily follow that the problem of finding the probabilities $\Phi(X_i^{(1)}|Y_j^{(1)}G_j^{(1)})$ is *similar* to that of finding the probabilities $\Phi(X_i^{(2)}|Y_j^{(2)}G_j^{(2)})$.

5.2 The principle of indifference

This takes the following general form.

Principle of indifference

If on the basis of knowledge YG alone we are indifferent between the m mutually exclusive (but not necessarily exhaustive) claims of propositions A_j ($j = 1, \dots, m$), then under knowledge YG we should set our degrees of belief equal, i.e.

$$|\Phi(A_1|Y)|^2 = |\Phi(A_2|Y)|^2 = \dots = |\Phi(A_m|Y)|^2. \quad (5.2.1)$$

If in addition, the differences between the properties claimed by the A_j cannot be expressed *absolutely* using natural measures, natural orders or natural directions or other such concepts from knowledge YG , then under knowledge YG we are *absolutely indifferent* between the alternative propositions[†] and we should set our *phases* of belief equal also, so that

$$\Phi(A_1|Y) = \Phi(A_2|Y) = \dots = \Phi(A_m|Y). \quad (5.2.2)$$

* This form of the similarity principle is employed in section 9.2 of Chapter VI and in section 5 of Chapter IV.

† As noted in connection with the similarity principle this requires the propositions to be expressed *plainly* and to claim appropriate physical properties (not properties merely correlated with them).

Note that there is no general converse to the principle of indifference. So, for example, if (5.2.2) holds for mutually exclusive (and perhaps exhaustive) propositions A_j ($j = 1, \dots, m$) it does not follow that, under knowledge YG we are absolutely indifferent between the A_j . Without us being in a state of indifference, (5.2.1) or (5.2.2) might hold by accident or for some other reason. We do however make the following claim.

*Principle of indifference (cont.)**

If under knowledge G we are indifferent but not *absolutely indifferent* between propositions A and B under *any* state of knowledge Y of dynamical properties of the physical world, then there is at least one state of knowledge Y for which the probabilities A and B differ with regard to their phases so that

$$|\Phi(A|Y)|^2 = |\Phi(B|Y)|^2$$

(on account of our indifference) but

$$\Phi(A|Y) \neq \Phi(B|Y).$$

5.3 The method of transformation groups

The method is difficult to explain in general terms. It will become clear in applications. Briefly it consists of finding a group of transformations of propositions such that each transformation converts the problem of finding a probability distribution (or a number of probability distributions) into a *similar* problem such that the similarity principle (of section 5.1) and the uniqueness principles of probability assignment (beginning of section 5) can be employed to calculate the probability distribution(s) or at least to find a general form for the function(s) representing the distribution(s).

6. Relation to classical probability

It will be noted from (2.3.1) and (2.4.1) above that the *squared moduli* of the new (complex-valued) probabilities obey the sum rule and (under certain conditions) the product rule of *classical* probability theory. From section 5 we see that the squared moduli are also subject to the classical principles of probability assignment. So the new theory of probability reduces to or coexists with the classical theory of probability whenever we know (from G) that our knowledge is so limited (i.e. so approximate) that it is never pure and never restricted (to a significant extent) by the uncertainty principle. Then the product rule (2.4.1) always applies. And our probabilities are always

* This final part of the principle of indifference is employed in section 4.2 of Chapter X

probabilities of disjunctions of propositions claiming properties are quantified by numbers that are nearly the same (i.e. the same to classical accuracy). By the sum rule (2.3.1) they therefore have indeterminate phases. Phases of belief and of implication, and characteristic phases then lose significance and have no bearing on the calculation of the squared moduli of the probabilities. The phases can then simply be ignored or dropped and the squared moduli of the probabilities give degrees of belief satisfying all the rules of classical probability.*

Conversely, if classical probabilities $P(X_j|Y)$ $j=1,2,\dots$ have been *legitimately* calculated using the classical laws of probability and the classical rules for probability assignment, they may be converted into their complex-valued probability forms by taking their square roots and multiplying them by indeterminate phase factors. That is we should put (for all j)

$$\Phi(X_j|Y) = \sqrt{P(X_j|Y)}e^{i\alpha_j}$$

the real numbers α_j being indeterminate[†] and unrelated.

7. Principle of maximum entropy

In situations in which classical probability theory coexists with complex-valued probability theory (see section 6) we have the following additional principle of probability assignment.

The principle of maximum entropy

If $\Phi(X_i|Y)$ is our probability distribution for a finite set of mutually exclusive and exhaustive propositions X_i ($i=1,\dots,n$) the extent of our ignorance regarding which one of the X_i is true is measured by the ‘information entropy’ (or ‘entropy’ for short) given by

* Under these conditions *cognitive* independence of propositions is of course always present and *logical* independence (which may sometimes be present) is redefined as follows. Under conditions in which complex-valued probability and classical probability coexist, propositions A_1, A_2, \dots, A_m are logically independent under knowledge Y if and only if

$$|\Phi(A_1 A_2 \dots A_m | Y)|^2 = |\Phi(A_1 | Y)|^2 |\Phi(A_2 | Y)|^2 \dots |\Phi(A_m | Y)|^2.$$

† If, for some j , Y and X_j are one and the same proposition or claim exactly the same (classical)

physical property in a similar logical manner so that $Y \stackrel{0}{\Leftrightarrow} X_j$, then we should of course put

$\Phi(X_j|Y) = 1$, i.e. α_j is then determinate and equal to zero. But this exception is of no consequence.

$$S = -\sum_{i=1}^n |\Phi(X_i|Y)|^2 \ln |\Phi(X_i|Y)|^2 \quad (7.1)$$

and if knowledge Y (or rather YG) amounts to knowledge of one or more known constraints on the degree of belief distribution $|\Phi(X_i|Y)|^2$, then the probability distribution we should rationally hold is $|\Phi(X_i|Y)|e^{i\alpha_i}$ where the α_i are indeterminate and $|\Phi(X_i|Y)|^2$ is the degree of belief distribution that maximises S subject to the constraints*.

8. The possibility of wave function conjugation and its implications

We have said that under any pure state of knowledge the corresponding wave function (a probability distribution over a chosen basis) is calculable at least to within an indeterminate constant phase factor.

But as things stand this is not exactly true. Under pure knowledge, application of the laws of probability and the principles of probability assignment always result only in showing that a wave function *or its conjugate* must represent our knowledge. This is because all the laws of probability and the principles of probability assignments are satisfied just as well by the conjugates of all the probabilities (with changes (in sign) made also to related characteristic phases and phases of implication).

In order to fix a wave function (at least to within a constant phase factor) we have to make a choice between adopting a certain wave function or its conjugate. This is not an independent decision for each wave function because wave functions are often related (for example by Feynman's law). So in adopting a certain wave function (and not its conjugate) we must ensure the choice is consistent with choices already made with regard to related wave functions.

Looked at another way, each calculated wave function contains an unknown parameter λ multiplying every i (i.e. every square root of -1) in that wave function. The λ in each wave function is equal to $+1$ or to -1 . Rather than leave the λ s indeterminate we choose to fix them in a conventional way in certain (independent) wave functions and then deduced them for the others on the basis of the necessary relations between wave functions.

* One of the constraints is of course that $\sum_{i=1}^n |\Phi(X_i|Y)|^2 = 1$, but there may be others. And in the case i is a continuous parameter (over some range) with a natural measure, the principle of maximum entropy still applies with X_i denoting the proposition that i lies in one or other of a large number of small elements of equal measure filling the range. (See p. 375 of [2].)

8.1 Implications for the similarity principle under pure knowledge

The possibility of wave function conjugation has implications with regard to the similarity principle (5.1.2) of section 5.1. As it stands, the similarity principle there implies that if we have to find the wave function over a basis $x_i^{(1)}$ of a complete sample space under various pure states of knowledge $Y_j^{(1)}G_j^{(1)}$ and if this problem is recognisably *similar* to one of finding the wave function over a basis $x_i^{(2)}$ of the same sample space under pure states of knowledge $Y_j^{(2)}G_j^{(2)}$, then for each i and j we should set

$$\Phi(x_i^{(1)}|Y_j^{(1)}G_j^{(1)}) = \Phi(x_i^{(2)}|Y_j^{(2)}G_j^{(2)})e^{i\alpha} \quad (8.1.1)$$

where α is some real constant independent of i and j . On account of the possibility of wave function conjugation, however, it would seem reasonable to propose instead that

$$\Phi(x_i^{(1)}|Y_j^{(1)}G_j^{(1)}) = \Phi^*(x_i^{(2)}|Y_j^{(2)}G_j^{(2)}) \quad (8.1.2)$$

for all i and j . That is, instead of the relations (8.1.1), the wave functions in case (1) might be the conjugates of the wave functions in case (2). We do in fact adopt this possibility as an extension of the principle of similarity. So according to the principle of similarity in its full form, either (8.1.1) *or* (8.1.2) must hold when the problems of finding the wave functions in cases (1) and (2) are recognisably similar.*

We note however that in applications of the similarity principle to calculate wave functions, use of (8.1.2) rather than (8.1.1) is seldom possible. This is because we assume wave functions must be differentiable functions of their continuous variables *and* of any continuous parameters in them. This logical requirement excludes (8.1.2) whenever we can pass from case (1) to case (2) by making infinitesimal changes in continuous parameters with similarity applying in each step. But when we cannot pass from case (1) to case (2) in that manner, (8.1.2) becomes a possibility while a relation of the kind (8.1.1) might be untenable.

Of course the possibility of conjugation applies not just to wave functions but to *any* probability distributions calculated using the laws of probability and the principles of probability assignments. Taking the conjugate of all calculated probabilities (and changing the sign of all related phases of implication, and characteristic phases) still results in agreement with those laws and principles. Therefore the general extension of the similarity principle (5.1.2) is expressed by allowing, under similarity, either (8.1.1) or (8.1.2) where $x_i^{(1)}$ and $x_i^{(2)}$ may stand for more general propositions $X_i^{(1)}$ and $X_i^{(2)}$ of

* We stress that either (8.1.1) *or* (8.1.2) must then apply for all j (as well as for all i). We do not allow that under similarity (8.1.1) might hold for some j values while (8.1.2) holds for the others.

equal number (not just propositions of bases of a complete sample space). And $Y_j^{(1)}$ and $Y_j^{(2)}$ may represent states of knowledge that are not necessarily pure.

As noted already (in section 5.1) a similarity principle has no converse. So if (8.1.2) is true (in bases $x_i^{(1)}$ and $x_i^{(2)}$) for a set of propositions $Y_j^{(1)}G_j^{(1)}$, and an equally numerable set of propositions $Y_j^{(2)}G_j^{(2)}$ it does not necessarily follow that the problems of finding wave functions $\Phi(x_i^{(1)}|Y_j^{(1)}G_j^{(1)})$ is *similar* to that of finding wave functions $\Phi(x_i^{(2)}|Y_j^{(2)}G_j^{(2)})$.

It is true that if problem (1) is *similar* to problem (2) then problem (2) is *similar* to problem (1). But if problem (1) is *similar* to problem (2) and problem (2) is *similar* to problem (3), it does not necessarily follow that problem (1) is *similar* to problem (3).*

Throughout most of our work we will apply the similarity principles in their original forms (as in section 5.1) and make no reference to the above extension. This is just because of the above mentioned requirement for differentiability of wave functions which usually rules out (8.1.2) (as may easily be checked in detail on each occasion). We will however need to take account of the above extension in the cases of discrete transformation groups (applied, for example, in relation to time reversal or inversion).

8.2 Implications for the first law of extreme values of probability

The possibility of wave function conjugation (or rather conjugation of any probability distribution), must of course, when applied, be accompanied by a change in sign of related characteristic phases and phases of implication (whether these take determinate values or not).

A consequence of this is that no (non-zero) phase of implication α has a determinate value and at best is determined only to within a factor of ± 1 .

This might be thought to affect the first law of extreme values of probability (in section 2.2.2) because, strictly speaking, the phases referred to in that law *never* have determinate values.† However, with the understanding that we always make a definite choice between a wave function (or probability distribution) and its conjugate (as we always do) and accordingly make a definite choice of the sign of any associated phase of implication, the law as originally stated in section 2.2.2 is true enough and can stay as it is. Or, put another way, the law is true enough as it stands so long as we count as ‘determinate’ any phase which is indeterminate (in sign) only because of the possibility of wave function (or probability distribution) conjugation, and we count as

* If (8.1.1) is the consequence of *similarity* of cases (1) and (2) and

$\Phi(X_i^{(2)}|Y_j^{(2)}G_j^{(2)}) = \Phi^*(X_i^{(3)}|Y_j^{(3)}G_j^{(3)})$ the consequence of *similarity* of cases (2) and (3) it is

certainly not the case that cases (1) and (3) are *similar*.

† Any one of them has of course a determinate value when it is zero, but this covers only very special cases.

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‘indeterminate’ only phases which are indeterminate for reasons other than the arbitrariness of their signs under wave function (or probability distribution) conjugation.

CHAPTER II

CONSEQUENCES OF THE LAWS OF COMPLEX-VALUED PROBABILITY

1. General consequences

We begin by noting the following rule.

The second addition rule for phases characteristic of knowledge

If the phase characteristic of knowledge Y is k and if $Y \stackrel{-\gamma}{\Leftrightarrow} Y'$ then the phase characteristic of knowledge Y' is $k + \gamma$.

We call it the *second* addition rule to distinguish it from the first addition rule for phases characteristic of knowledge declared in section 2.4 of Chapter I.

The second rule for phases characteristic of knowledge follows easily from the general rule for phases (section 5 of Chapter I). For if $Y \stackrel{-\gamma}{\Leftrightarrow} Y'$ then the general expression ((2.2.1.8) of Chapter I) for the probability of A under knowledge Y gives

$$\Phi(A|Y') = \Phi(A|Y)e^{-i\gamma} = \sqrt{|\Phi(A|Y)|^2} e^{i(\chi - (k + \gamma))}$$

and on account of (2.2.1.10) of Chapter I, $k + \gamma$ must be the phase characteristic of knowledge Y' .

We next note the following rule.

The rule for phases characteristic of propositions under knowledge

If the characteristic phase of A under knowledge Y is $\text{ch}(A|Y)$ and if $A \stackrel{-\alpha}{\Leftrightarrow} A'$, then the characteristic phase of A' under knowledge Y is $\text{ch}(A|Y) + \alpha$. i.e.

$$\text{ch}(A'|Y) = \text{ch}(A|Y) + \alpha \quad (1.1)$$

This rule is also a simple consequence of the general rule for phases and the general form ((2.2.1.8) of Chapter I) of a probability. And because characteristic phases under knowledge stay the same under an equivalence transformation of knowledge we have

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$$\text{ch}(A'|Y') = \text{ch}(A|Y) + \alpha \quad (1.2)$$

when $A \stackrel{-\alpha}{\Leftrightarrow} A'$ and $Y \stackrel{-\gamma}{\Leftrightarrow} Y'$.

Finally we note that by putting A equal to Y in (2.2.1.20) of Chapter I we establish the relation

$$Y \stackrel{-k}{\Leftrightarrow} YY \quad (1.3)$$

where k is the phase characteristic of Y . Thus given any proposition Y which claims a dynamical property and could represent a state of knowledge, the phase k characteristic of knowledge Y is the same as the phase of implication of YY by Y .

We now go on to demonstrate other consequences (of the laws of complex-valued probability) under various headings.

1.1 The invariance of general probability relations under equivalence

Any *general* relation between the probabilities of propositions about the physical world will be invariant under equivalence. For if

$$A \stackrel{-\alpha}{\Leftrightarrow} A', B \stackrel{-\beta}{\Leftrightarrow} B', \dots \text{etc}, \quad (1.1.1)$$

and any one general relation between the probabilities of the propositions A, B, \dots is transformed (using the general rule for phases (section 5 of Chapter I)) into another (derived) relation between the probabilities A', B', \dots , then, since the original relation (between the A, B, \dots) is a *general* relation it must hold also for the propositions A', B', \dots . So the derived relation can only be the same as the original relation.

We demonstrate this invariance in a number of examples.

Example 1. The product rule

Let us start out with the product rule

$$\Phi(AB|Y) = \Phi(A|Y)\Phi(B|AY)e^{i(k+\varepsilon)} \quad (1.1.2)$$

where the real numbers k and ε are the phases characteristic of knowledge Y and of knowledge A respectively. This rule holds only when A and B claim compatible properties and A represents a possible state of knowledge that can be held in conjunction with knowledge Y . We will denote this condition as:

$$[A, B|A, Y] \quad (1.1.3)$$

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which reads ‘ A and B claim compatible properties and, A and Y represent compatible states of knowledge’.

Now suppose

$$A^{-\alpha} \Leftrightarrow^{\alpha} A', \quad B^{-\beta} \Leftrightarrow^{\beta} B', \quad Y^{-\gamma} \Leftrightarrow^{\gamma} Y' \quad (1.1.4)$$

then by the rule of phase addition under conjunction (first of (2.2.1.7) of Chapter I)

$$AB^{-\alpha-\beta} \Leftrightarrow^{\alpha+\beta} A'B', \quad AY^{-\alpha-\gamma} \Leftrightarrow^{\alpha+\gamma} A'Y' \quad (1.1.5)$$

and applying the general rule for phases (section 5 of Chapter I) (1.1.2) becomes

$$\Phi(A'B'|Y')e^{-i(\alpha+\beta)}e^{i\gamma} = \Phi(A|Y')e^{-i\alpha}e^{i\gamma} \cdot \Phi(B'|A'Y')e^{-i\beta}e^{i(\alpha+\gamma)}e^{i(k+\varepsilon)}$$

or

$$\Phi(A'B'|Y') = \Phi(A|Y')\Phi(B'|A'Y')e^{i((k+\gamma)+(\varepsilon+\alpha))} \quad (1.1.6)$$

But by the second addition rule for phases characteristic of knowledge $k+\gamma$ is the characteristic phase k' characteristic of knowledge Y' and $\varepsilon+\alpha$ is the phase ε' characteristic of knowledge A' so that

$$\Phi(A'B'|Y') = \Phi(A|Y')\Phi(B'|A'Y')e^{i(k'+\varepsilon')}$$

which is exactly the same relation between A' , B' and Y' as (1.1.2) was between A , B and Y .

Example 2. The logical independence relation

The relation (2.5.1) of Chapter I expressing logical independence of A and B under knowledge Y becomes, under (1.1.4),

$$\Phi(A'B'|Y') = \Phi(A|Y') \cdot \Phi(B'|Y')e^{ik'}$$

where $k' = k + \gamma$ and this result shows that A' and B' are logically independent under knowledge Y' whenever A and B are logically independent under knowledge Y .

Example 3. The sum rule

The generalised sum rule ((2.3.2) of Chapter I) is

$$\Phi(A+B+\dots|Y) = e^{i(\eta-k)} \sqrt{|\Phi(A|Y)|^2 + |\Phi(B|Y)|^2 + \dots}$$

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where k is the phase characteristic of knowledge Y and η the (usually indeterminate) phase characteristic of the disjunction $A+B+\dots$ under knowledge Y . It holds under any knowledge Y whenever propositions A, B, \dots are mutually exclusive.

Under the transformation $A^{-\alpha} \Leftrightarrow^{\alpha} A'$, $B^{-\beta} \Leftrightarrow^{\beta} B', \dots$ and $Y^{-\gamma} \Leftrightarrow^{\gamma} Y'$ the general rule for phases clearly leaves the square root term unchanged, and since

$$A + B + \dots \Leftrightarrow^{\varepsilon} A' + B' + \dots$$

with some phase of implication ε , we have

$$\Phi(A' + B' + \dots | Y') = e^{i(\eta + \varepsilon - (k + \gamma))} \sqrt{|\Phi(A' | Y')|^2 + |\Phi(B' | Y')|^2 + \dots}$$

where, by the second rule for phases characteristic of knowledge, $k + \gamma$ is the phase k' characteristic of knowledge Y' , and by the rule for phases characteristic of propositions under knowledge, $\eta + \varepsilon$ is the phase η' characteristic of $A' + B' + \dots$ under knowledge Y' . So we have derived

$$\Phi(A' + B' + \dots | Y') = e^{i(\eta' - k')} \sqrt{|\Phi(A' | Y')|^2 + |\Phi(B' | Y')|^2 + \dots}$$

which is exactly the same relation between A', B', \dots and Y' as the original relation was between A, B and Y .

Example 4. The similarity relation (5.1.3) of Chapter I

Since this particular similarity relation is supposed to hold for *any* propositions Y_j and $Y_{j'}$ which could represent our knowledge of dynamical properties it must be invariant under an equivalence transformation $Y_j^{-\lambda_j} \Leftrightarrow^{\lambda_j} Y_{j'}$ where the phase of implication may vary with j in any possible way. By the general rule for phases and the second addition rule for phases characteristic of knowledge this is clearly the case.

Example 5. Feynman's Law

In the more general form of Feynman's Law ((3.5.2) of Chapter I) Z and Y are general enough propositions for invariance under equivalence to hold. For if $Z^{-\xi} \Leftrightarrow^{\xi} Z'$ and $Y^{-\gamma} \Leftrightarrow^{\gamma} Y'$ where ξ and γ may or may not be determinate, the propositions Z' and Y' might represent pure states of knowledge just as well as the propositions Z and Y are supposed to do. We therefore expect (3.5.2) of Chapter I to be invariant under $Z^{-\xi} \Leftrightarrow^{\xi} Z'$ and $Y^{-\gamma} \Leftrightarrow^{\gamma} Y'$, and by the general rule for phases, this is clearly the case.

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Example 6. Laws relating to transformation functions

In the laws (3.4.1)-(3.4.9) of Chapter I relating to transformation functions the propositions x_i and y_j are not *general* propositions—they are propositions of *bases*. And under a general equivalence transformation $x_i^{-\alpha_i} \Leftrightarrow^{\alpha_i} x'_i, y_j^{-\beta_j} \Leftrightarrow^{\beta_j} y'_j$ we cannot claim x'_i and y'_j also constitute bases. This will be so only under certain conditions. In the first place the relative phases α_i must be determinate and the same must apply to the β_j , so that the new transformation functions $\Phi(x'_i|y'_j)$ have determinate relative phases.

Under this condition alone, Chapter I equations (3.4.1), (3.4.3), (3.4.4), (3.5.1) and (3.5.2), are, by the general rule for phases, clearly invariant under the equivalence transformation $x_i^{-\alpha_i} \Leftrightarrow^{\alpha_i} x'_i, y_j^{-\beta_j} \Leftrightarrow^{\beta_j} y'_j$, where, in the case of (3.4.4) it must be understood that the necessary coefficients a_j change to $a'_j = a_j e^{i\beta_j}$.

But under the same condition (of determinate relative phases of the α_i and β_j) equation (3.4.2) of Chapter I is *not* invariant. For we find

$$\begin{aligned} \det[\Phi(x'_i|y'_j)] &= \begin{vmatrix} \Phi(x'_1|y'_1) & \Phi(x'_1|y'_2) & \dots \\ \Phi(x'_2|y'_1) & \Phi(x'_2|y'_2) & \dots \\ \dots & \dots & \dots \end{vmatrix} = \begin{vmatrix} e^{i(\alpha_1-\beta_1)}\Phi(x_1|y_1) & e^{i(\alpha_1-\beta_2)}\Phi(x_1|y_2) & \dots \\ e^{i(\alpha_2-\beta_1)}\Phi(x_2|y_1) & e^{i(\alpha_2-\beta_2)}\Phi(x_2|y_2) & \dots \\ \dots & \dots & \dots \end{vmatrix} \\ &= e^{i(\alpha_1+\alpha_2+\dots)-i(\beta_1+\beta_2+\dots)} \det[\Phi(x_i|y_j)] \end{aligned}$$

So other conditions required for the invariance of (3.4.2) of Chapter I are that

$$\left. \begin{aligned} \alpha_1 + \alpha_2 + \dots &= 0 \\ \beta_1 + \beta_2 + \dots &= 0 \end{aligned} \right\} \quad (1.1.7)$$

while (like x_i and y_j) the x'_i and y'_j form naturally ordered finite bases for $i = 1, 2, \dots, N$ and $j = 1, 2, \dots, N$.

The sum rule for transformation functions (as in (3.4.5)-(3.4.9) of Chapter I) is invariant under $x_i^{-\alpha_i} \Leftrightarrow^{\alpha_i} x'_i, y_j^{-\beta_j} \Leftrightarrow^{\beta_j} y'_j$ provided only that the condition for this sum rule (as in (3.4.6) of Chapter I) is maintained. For this to be the case it is necessary that α_i be the same for each member (x_4, x_7, \dots) of the disjunction, i.e. that

$$\alpha_4 = \alpha_7 = \dots = \alpha \quad (1.1.8)$$

so that, by the rule (1.2) for phases characteristic of propositions under knowledge, we have

$$\text{ch}(x'_4|y'_j) = \text{ch}(x_4|y_j) + \alpha$$

$$\text{ch}(x'_7|y'_j) = \text{ch}(x_7|y_j) + \alpha$$

...

which (like $\text{ch}(x_4|y_j), \text{ch}(x_7|y_j), \dots$) are all equal. Under (1.1.8), i.e. when $x_4^{-\alpha} \Leftrightarrow^{\alpha} x'_4$, $x_7^{-\alpha} \Leftrightarrow^{\alpha} x'_7, \dots$ the characteristic phase η'_j of $x'_4 + x'_7 + \dots$ under knowledge y'_j will be α plus the characteristic phase η_j of $x_4 + x_7 + \dots$ under knowledge y_j . (This follows from the *constancy of phase of implication between disjunctions of similarly equivalent propositions* (in section 2.2.1 of Chapter I) which results in $x'_4 + x'_7 + \dots^{-\alpha} \Leftrightarrow^{\alpha} x_4 + x_7 + \dots$) Hence $\eta'_j = \eta_j + \alpha = \text{ch}(x_4|y_j) + \alpha = \text{ch}(x'_4|y'_j)$, so the sum rule for transformation functions holds just as well for $x'_4 + x'_7 + \dots$ under knowledge y'_j as it did for $x_4 + x_7 + \dots$ under knowledge y_j , and claim (3.4.7) of Chapter I is invariant.

1.2 Consequences of logical identities

The pure logic rules of commutation and association, as expressed in (2.2.1.6) of Chapter I, have consequences as follows.

In relation to the sum rule

In the sum rule (2.3.2) of Chapter I the indeterminate phase η (or χ in (2.3.1) of Chapter I) must be the same regardless of the order or grouping of the mutually exclusive propositions A, B, \dots in the disjunction $A + B + \dots$ on the LHS. This is because, for example, $A + B \overset{0}{\Leftrightarrow} B + A$ so by the general rule for phases $\Phi(A + B|Y) = \Phi(B + A|Y)$ and χ in (2.3.1) of Chapter I must be the same for $\Phi(A + B|Y)$ as it is for $\Phi(B + A|Y)$.

In relation to the product rule

Since $AB \overset{0}{\Leftrightarrow} BA$ the product rule ((2.4.1) of Chapter I) implies

$$\Phi(AB|Y) = \Phi(A|Y)\Phi(B|AY)e^{i(k+\varepsilon)} = \Phi(B|Y)\Phi(A|BY)e^{i(k+\delta)}$$

so long as $[A, B|A, Y]$ and $[B, A|B, Y]$, where k, ε and δ are phases characteristic of knowledge Y, A and B respectively. We thus arrive at the form of Bayes' rule in complex-valued probability which states that provided $[A, B|A, Y]$ and $[B, A|B, Y]$ then

$$\Phi(A|BY) = \Phi(B|AY) \frac{\Phi(A|Y)e^{i\varepsilon}}{\Phi(B|Y)e^{i\delta}} \quad (1.2.1)$$

We also see that because of the commutation rule $AB \overset{0}{\Leftrightarrow} BA$ and the association rule $A(BC) \overset{0}{\Leftrightarrow} (AB)C$ the generalisation (2.4.2) (in Chapter I) of the product rule is derivable from the simple product rule (2.4.1) in Chapter I. The order or grouping of the factors A_1, A_2, \dots, A_m on the LHS of (2.4.2) of Chapter I is immaterial, so, for example we can derive (2.4.2) of Chapter I in the case $m=3$ using the forms

$$\begin{aligned} \Phi((A_1A_2)A_3|Y) &= \Phi(A_1A_2|Y)\Phi(A_3|A_1A_2Y)e^{i(k+\varepsilon_1+\varepsilon_2)} \\ \Phi(A_1A_2|Y) &= \Phi(A_1|Y)\Phi(A_2|A_1Y)e^{i(k+\varepsilon_1)} \end{aligned}$$

of (2.4.1) of Chapter I, where the first addition rule for phases characteristic of knowledge has been used in relation to knowledge A_1A_2 . Substituting the second form into the first gives

$$\Phi(A_1A_2A_3|Y) = \Phi(A_1|Y)\Phi(A_2|A_1Y)\Phi(A_3|A_1A_2Y)e^{i(2k+2\varepsilon_1+\varepsilon_2)}$$

which is (2.4.2) of Chapter I with $m=3$.

1.3 Consequences in relation to the product rule and the definition of logical independence

A consequence of the product rule ((2.4.1) of Chapter I) and the definition of logical independence ((2.5.1) of Chapter I) is as follows. In case $[A, B|A, Y]$, and A and B are logically independent of each other under knowledge Y , we have

$$\Phi(AB|Y) = \Phi(A|Y)\Phi(B|AY)e^{i(k+\varepsilon)} = \Phi(A|Y)\Phi(B|Y)e^{ik}$$

and therefore

$$\Phi(B|AY) = \Phi(B|Y)e^{-i\varepsilon}. \quad (1.3.1)$$

where ε is the phase characteristic of knowledge A . So, as in classical probability, given logical independence of A and B under knowledge Y (and given $[A, B|A, Y]$) our degree of belief in B is not changed on learning the truth of A . Note however that because of the need for the phase factor we are unable to claim $\Phi(B|AY) = \Phi(B|Y)$ in place of (1.3.1), but a consequence of (1.3.1) is the simple result

$$\text{ch}(B|AY) = \text{ch}(B|Y) \quad (1.3.2)$$

The results (1.3.1) and (1.3.2) clearly apply to any two propositions A and B taken from a set of three or more propositions (logically independent of each other under knowledge Y) whenever $[A, B|A, Y]$ applies to any pair A and B drawn from the set. Our degree of belief in any one (as well as its characteristic phase under knowledge Y) is then not changed on learning the truth of any other.

It follows from definition of logical independence ((2.5.1) of Chapter I) that if $Y \Rightarrow A$ and $Y \Rightarrow B$ then (as is trivially the case in classical probability) A and B are necessarily logically independent under knowledge Y .

For if $Y \Rightarrow^\alpha A$ and $Y \Rightarrow^\beta B$ then $YY \Rightarrow^{\alpha+\beta} AB$ and since $Y \Rightarrow^k YY$ we have $Y \Rightarrow^{\alpha+\beta+k} AB$ so that $\Phi(AB|Y) = \Phi(A|Y)\Phi(B|Y)e^{ik}$ which means A and B are logically independent under knowledge Y .

1.4 Consequences of the product rule

From the general form ((2.2.1.8) of Chapter I) of a probability we see that the product rule

$$\Phi(AB|Y) = \Phi(A|Y)\Phi(B|AY)e^{i(k+\varepsilon)} \quad (1.4.1)$$

entails the relation

$$\text{ch}(AB|Y) = \text{ch}(A|Y) + \text{ch}(B|AY) \quad (1.4.2)$$

under the condition $[A, B|A, Y]$ of course.

If in (1.4.1) we make B the same as Y (we sometimes write $B=Y$ in making such a substitution) we obtain

$$\Phi(AY|Y) = \Phi(A|Y)\Phi(Y|AY)e^{i(k+\varepsilon)}$$

provided $[A, Y|A, Y]$. Since $AY \Rightarrow^{-\varepsilon} Y$ (as follows from (2.2.1.21) of Chapter I) this gives the rule

$$\Phi(AY|Y) = \Phi(A|Y)e^{ik} \quad (1.4.3)$$

when $[A, Y|A, Y]$.

If in (1.4.1) we put $Y = AY$ we obtain

$$\Phi(AB|AY) = \Phi(A|AY)\Phi(B|AAY)e^{i(k+2\varepsilon)}$$

because the phase characteristic of knowledge AY is $k + \varepsilon$. Since $AA Y^\varepsilon \Leftrightarrow {}^{-\varepsilon}AY$ and $AY \Rightarrow {}^{-k}A$ this becomes

$$\Phi(AB|AY) = \Phi(B|AY)e^{i\varepsilon} \quad (1.4.4)$$

valid when $[A, B|A, AY]$. If in addition $Y \Rightarrow A$ then $AY^\varepsilon \Leftrightarrow {}^{-\varepsilon}Y$ (see (2.2.1.20) of Chapter I) and (1.4.4) gives

$$\Phi(AB|AY) = \Phi(B|Y) \quad (1.4.5)$$

valid when $[A, B|A, AY]$ and $Y \Rightarrow A$.

Finally, if in (1.4.1) we put $A = B$ we find

$$\text{ch}(A|AY) = \text{ch}(A) \quad (1.4.6)$$

when $[A, A|A, Y]$.

2. Product rule in a combination of logically independent sample spaces

Suppose we have M separate sample spaces $S^{(1)}, \dots, S^{(M)}$ all logically independent of each other under knowledge Y . If $X_i^{(1)}$ ($i=1, \dots, n^{(1)}$) are $n^{(1)}$ mutually exclusive (but not necessarily exhaustive) propositions of $S^{(1)}$, and $X_j^{(2)}$ ($j=1, \dots, n^{(2)}$) are $n^{(2)}$ mutually exclusive (but not necessarily exhaustive) propositions of $S^{(2)}$, and so on, then the propositions $X_i^{(1)}, \dots, X_l^{(M)}$ will be logically independent of each other under knowledge Y and therefore, by the definition of logical independence (2.5.2) of Chapter I we will have

$$\Phi(X_i^{(1)} \dots X_l^{(M)}|Y) = \Phi(X_i^{(1)}|Y) \dots \Phi(X_l^{(M)}|Y)e^{ik(M-1)} \quad (2.1)$$

If the $S^{(1)}, \dots, S^{(M)}$ are closed and contemporary, if knowledge Y amounts to pure states of knowledge $Y^{(1)}, \dots, Y^{(M)}$ in relation to each sample space (so that $Y = Y^{(1)} \dots Y^{(M)}$), and if the $X_i^{(1)}, \dots, X_l^{(M)}$ are propositions $x_i^{(1)}, \dots, x_l^{(M)}$ from contemporary bases in the respective sample spaces, then (2.1) becomes

$$\Phi(x_i^{(1)}, \dots, x_l^{(M)}|Y^{(1)} \dots Y^{(M)}) = \Phi(x_i^{(1)}|Y^{(1)} \dots Y^{(M)}) \dots \Phi(x_l^{(M)}|Y^{(1)} \dots Y^{(M)})e^{ik(M-1)} \quad (2.2)$$

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where k is the phase characteristic of knowledge $Y^{(1)} \dots Y^{(M)}$. In (2.2) i, j, \dots, l take values $i = 1, \dots, N^{(1)}, j = 1, \dots, N^{(2)}, \dots, l = 1, \dots, N^{(M)}$, where $N^{(1)}, N^{(2)}, \dots, N^{(M)}$ are the orders of the samples spaces $S^{(1)}, S^{(2)}, \dots, S^{(M)}$.

The result (2.2) is different from the product rule for wave functions (section 3.7 of Chapter I). The factors $\Phi(x_i^{(1)}|Y^{(1)} \dots Y^{(M)}), \dots, \Phi(x_l^{(M)}|Y^{(1)} \dots Y^{(M)})$ on the RHS of (2.2) differ (with regard to their absolute phases) from the wave functions $\Phi(x_i^{(1)}|Y^{(1)}), \dots, \Phi(x_l^{(M)}|Y^{(M)})$ in each sample space. But we will generally have that

$$\left. \begin{aligned} \Phi(x_i^{(1)}|Y^{(1)} \dots Y^{(M)}) &= \Phi(x_i^{(1)}|Y^{(1)})e^{i\alpha^{(1)}} \\ \Phi(x_j^{(2)}|Y^{(1)} \dots Y^{(M)}) &= \Phi(x_j^{(2)}|Y^{(2)})e^{i\alpha^{(2)}} \\ \dots \text{etc.} \end{aligned} \right\} \quad (2.3)$$

where $\alpha^{(1)}, \alpha^{(2)}, \dots$ are certain phases independent of i, j, \dots . Equating the RHS of (2.2) to the product $\Phi(x_i^{(1)}|Y^{(1)}) \dots \Phi(x_l^{(M)}|Y^{(M)})$ of the wave functions (as we may on account of the product rule for wave functions) we obtain (by (2.3)) the necessary relation

$$\alpha^{(1)} + \alpha^{(2)} + \dots + \alpha^{(M)} + k(M-1) = 0. \quad (2.4)$$

Note that (2.2) (as a relation between probabilities) is true (i.e. a consequence of (2.1)) also when the sample spaces and/or the bases $x_i^{(1)}, \dots, x_l^{(M)}$ are *not* contemporary* and the normal product rule for wave functions does not apply.

3. Separability of degree of belief distributions when joint distributions factor

Let sample spaces $S^{(1)}$ and $S^{(2)}$ be separate and let $X_i^{(1)}$ and $X_j^{(2)}$ respectively be sets of mutually exclusive and exhaustive propositions in each. Now suppose that under knowledge Y in relation to $S^{(1)}S^{(2)}$ our degree of belief distribution $|\Phi(X_i^{(1)}X_j^{(2)}|Y)|^2$ factors thus

$$|\Phi(X_i^{(1)}X_j^{(2)}|Y)|^2 = f_i g_j$$

* This fact is of relevance in connection with the use of (2.1) in section 9. For it implies the frequency rule (of section 9) applies when the $X_i^{(r)}$ ($r = 1, \dots, M$) there are non-contemporary bases $x_i^{(r)}$ in contemporary or non-contemporary sample spaces $S^{(r)}$ $r = 1, \dots, M$.

where f_i and g_j are positive and normalised distributions over i and j respectively. Then since $X_i^{(1)}$ is equivalent to $X_i^{(1)}(X_1^{(2)} + X_2^{(2)} + \dots)$ or to $X_i^{(1)}X_1^{(2)} + X_i^{(1)}X_2^{(2)} + \dots$ we have by the sum rule ((2.3.2) of Chapter I) that

$$|\Phi(X_i^{(1)}|Y)|^2 = \sum_j |\Phi(X_i^{(1)}X_j^{(2)}|Y)|^2 = \sum_j f_i g_j = f_i \sum_j g_j = f_i$$

and similarly

$$|\Phi(X_j^{(2)}|Y)|^2 = g_j$$

so that the factors f_i and g_j give the separate degree of belief distributions in the each sample space. This property extends naturally to the case of any number of separate sample spaces.

4. Wave function after harmless conditioning

Given a representation of a pure state by a wave function $\Phi(x_i|Y)$ $i = 1, \dots, N$ using any *primary* basis x , we can by chance (as we have said in section 3.6 of Chapter I), instantly get to know the truth of a proposition A which is the disjunction of a set A of the propositions x_i . And the acquisition of knowledge A can be achieved by chance without affecting the truth values of the x_i or invalidating our knowledge Y . Then our knowledge changes to AY representing a new pure state of knowledge with wave function $\Phi(x_i|AY)$.

Harmless acquisition of knowledge A will of course affect the *probabilities* of the x_i . In fact, because condition $[x_i, A|A, Y]$ holds when $x_i \in A$, the product rule gives us

$$\Phi(x_i A|Y) = \Phi(A|Y)\Phi(x_i|AY)e^{i(k+\varepsilon)} \quad (4.1)$$

where k and ε are the phases characteristic of knowledge Y and A respectively. Since we assume $\Phi(A|Y) \neq 0$ we have (for $x_i \in A$)

$$\Phi(x_i|AY) = \frac{\Phi(x_i A|Y)}{\Phi(A|Y)} e^{-i(k+\varepsilon)}$$

But when $x_i \in A$ we have $x_i \Rightarrow A$, and by the general rule (2.2.1.20) of Chapter I, we have $x_i^{-\varepsilon} \Leftrightarrow^\varepsilon x_i A$, making

$$\Phi(x_i|AY) = \frac{\Phi(x_i|Y)e^{i\epsilon}}{\Phi(A|Y)} e^{-i(k+\epsilon)}$$

and since $\Phi(x_i|AY)$ is clearly zero when $x_i \notin A$, we arrive at

$$\Phi(x_i|AY) = \begin{cases} \frac{\Phi(x_i|Y)}{\Phi(A|Y)} e^{-ik} & x_i \in A \\ 0 & x_i \notin A \end{cases} \quad (4.2)$$

After harmless conditioning the relative moduli and relative phases of the probabilities remain the same for propositions x_i in the set A , and the moduli become zero for the propositions x_i outside the set A .*

If A contains only one proposition x_i then (4.2) gives

$$\Phi(x_i|AY) = e^{-ik} \delta_{il} \quad (\text{when } A = x_i) \quad (4.3)$$

where the phase k characteristic of knowledge Y is an indeterminate phase.

If A contains *all* the propositions x_i for $i=1,2,\dots,N$ then A claims knowledge of a dynamical property known to be present under our general knowledge G . Therefore $\Phi(A|Y) = e^{-ik}$ (as in (2.3.3) of Chapter I) and by (4.2) our wave function undergoes no change at all, i.e. $\Phi(x_i|AY)$ is the same as $\Phi(x_i|Y)$.

5. The product rule for transformation functions or Feynman's law in a combination of closed sample spaces

As we said in section 3.7 of Chapter I, a number M of contemporary and closed sample spaces $S^{(1)}, \dots, S^{(M)}$ (referring to distinct systems) with respective bases $x_i^{(1)}, \dots, x_i^{(M)}$ all pertaining to the same time t can be combined to form a closed sample space $S = S^{(1)} \dots S^{(M)}$ with a basis $x_i^{(1)} \dots x_i^{(M)}$ (pertaining to time t) with respect to which pure states of knowledge may be expressed.

Bases in S can be formed in more than one way depending on the choice of the bases in each component sample space. If knowledge Y pure in relation to S is represented by the wave function $\Phi(x_i^{(1)} \dots x_i^{(M)}|Y)$ and by a wave function $\Phi(y_i^{(1)} \dots y_i^{(M)}|Y)$

* An example of harmless conditioning, is the filtering of spin components using a Stern-Gerlach apparatus (see section 5-1 of [7]). And notional methods for accomplishing harmless conditioning with regard to particle position and particle spin are modelled in Chapter XIII.

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using alternative bases $y_i^{(1)}, \dots, y_i^{(M)}$ all pertaining to (a possibly different) time t' , the question arises as to how these wave functions are related.

It follows from the product rule for wave functions (section 3.7 of Chapter I) that the transformation functions connecting $\Phi(x_i^{(1)} \dots x_i^{(M)} | Y)$ and $\Phi(y_i^{(1)} \dots y_i^{(M)} | Y)$, i.e. the wave functions $\Phi(x_i^{(1)} \dots x_i^{(M)} | y_i^{(1)} \dots y_i^{(M)})$, are the products of the transformation functions $\Phi(x_i^{(1)} | y_i^{(1)})$, \dots , $\Phi(x_i^{(M)} | y_i^{(M)})$ in $S^{(1)}, \dots, S^{(M)}$ respectively, so that Feynman's law in S takes the form

$$\Phi(x_i^{(1)} \dots x_i^{(M)} | Y) = \sum_{i_j' \dots} \Phi(x_i^{(1)} | y_i^{(1)}) \dots \Phi(x_i^{(M)} | y_i^{(M)}) \Phi(y_i^{(1)} \dots y_i^{(M)} | Y). \quad (5.1)$$

In the case of just two sample spaces $S^{(1)}$ and $S^{(2)}$, with bases $x_j^{(2)}$ and $y_j^{(2)}$ the same*, so that $\Phi(x_j^{(2)} | y_j^{(2)}) = \delta_{jj'}$, Feynman's law (5.1) becomes

$$\Phi(x_i^{(1)} x_j^{(2)} | Y) = \sum_k \Phi(x_i^{(1)} | y_k^{(1)}) \Phi(y_k^{(1)} x_j^{(2)} | Y). \quad (5.2)$$

Feynman's law (5.1) for a combination of closed sample spaces (like Feynman's law (3.5.1) of Chapter I, for a single closed sample space) formally resembles the classical probability rule connecting distributions and (on account of the probabilities being complex) leads again to 'interference of probabilities'. It is also a more general quantitative expression of the uncertainty principle.

6. The association of properties with linear operators, and observations concerning the law of inferred dynamical properties

6.1 Association of bases and basic properties with complete sets of orthonormal wave functions

Given any known basis x_i in a sample space S , any other basis y_j in S is clearly associated with a certain complete set of orthonormal wave functions of i - namely the transformation functions $\phi_{ij} = \Phi(x_i | y_j)$ from basis y_j to basis x_i .

Now y_j is the proposition that a property P_{y_j} is possessed by the moving system under study, or that the basic property P_y is quantified by the parameter value j .

The parameter j is not unique. Suppose $j = f(j')$ is a 1-1 functional relation between parameter j and an alternative parameter j' . Then the proposition $y_{j'}$ that claims a value j' of the alternative parameter applies, is fully equivalent to the

* Of course this can apply only when $t' = t$.

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proposition y_j (where $j = f(j')$) and the transformation functions are, by the second uniqueness principle of section 5 Chapter I, the same. That is $y_j' \Leftrightarrow^0 y_j$ and

$$\Phi(x_i|y_j) = \Phi(x_i|y_j'),$$

when $j = f(j')$. A different choice of a parameter amounts only to quantifying the basic property P_y in a different way – e.g. in different units.

To every basis y_j there therefore corresponds a complete set of orthonormal functions $\phi_{ij} (= \Phi(x_i|y_j))$, the functions $\Phi(x_i|x_j) = \delta_{ij}$ corresponding to the basis x itself.

We are not claiming that to every complete set of orthonormal functions there corresponds a basis. However, given one basis x another basis y can be *postulated* in terms of transformation functions from y to x . That is, there is nothing stopping us claiming that a basis y (and therefore a basic property P_y of the moving system under study) exists with specified transformation functions $\Phi(x_i|y_j)$ to the known basis x .* The specified transformation functions must of course satisfy all the necessary properties of transformation functions in general and if we were to claim y was a *primary* basis it would be necessary to demonstrate the possibility of harmless conditioning over the y_j (see section 3.6 of Chapter I).

Starting with another (known) basis z_k , any new basis y_j may alternatively be associated with the transformation functions from y_j to z_k . In particular the original basis x_i is then specified by the transformation functions $\Phi(z_k|x_i)$ - i.e. by the complex conjugate of $\Phi(x_i|z_k)$. More generally the relation between two specifications $\Phi(z_k|y_j)$ and $\Phi(x_i|y_j)$ of a basis y_j is, by Feynman's law,

$$\Phi(z_k|y_j) = \sum_i \Phi(z_k|x_i)\Phi(x_i|y_j).$$

6.2 Association of basic properties with operators

With any basis y_j (or with its associated property P_y) we may associate a linear operator \hat{f} in the space of wave functions of i using a basis x_i . We define this operator by its effect on the transformation functions, thus for all j

* Such a claim amounts to a new physical law – that there is a basic property of the moving system under study besides those already known. Although we point out the possibility of specifying new bases in this way we have so far not needed to actually employ it.

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$$\hat{f}' \Phi(x_i|y_j) = j \Phi(x_i|y_j). \quad (6.2.1)$$

Because of the linearity of \hat{f} and the completeness of the transformation functions, (6.2.1) determines \hat{f} uniquely. The eigenvalues being always real, the operator \hat{f} is always Hermitian.

Using a new parameter j' where $j' = g(j)$ is a real valued 1-1 transformation, \hat{f} is supposed to transform to \hat{f}' defined by

$$\hat{f}' \Phi(x_i|y_{j'}) = j' \Phi(x_i|y_{j'})$$

or equivalently

$$\hat{f}' \Phi(x_i|y_j) = g(j) \Phi(x_i|y_j).$$

So we may formally write

$$\hat{f}' = g(\hat{f})$$

i.e. \hat{f}' is the same function of \hat{f} as j' is of j .

So however the parameter j is defined, the corresponding operator \hat{f} we associate with the basis y_j or with the property P_y always has the transformation functions $\Phi(x_i|y_j)$ as its eigenfunctions and the parameter j values as its eigenvalues.

Note that if j stands for M parameters needed to enumerate the propositions of the basis y or equivalently to quantify a M dimensional basic property P_y then \hat{f} stands for a *set* of linear operators, M in number. To be more specific, suppose j stands for j_1, \dots, j_M - i.e. for M independent real parameters, then \hat{f} stands for a set $\hat{f}_1, \dots, \hat{f}_M$ of operators satisfying

$$\hat{f}_k \Phi(x_i|y_j) = j_k \Phi(x_i|y_j), \quad k = 1, \dots, M$$

simultaneously. Or, if $j'_k = g_k(j_1, \dots, j_M)$ $k = 1, \dots, M$ is a 1-1 and real transformation, then $\hat{f}'_k = g_k(\hat{f}_1, \dots, \hat{f}_M)$ for $k = 1, \dots, M$. However the parameters j_k are defined, the corresponding operators \hat{f}_k clearly commute with one another and form a complete set, meaning that any linear operator that commutes with the \hat{f}_k can only be a function of them (see p.78 of [9]).

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The transformation functions from y_j to x_i specify the operator \hat{f} completely. But the converse is not true. Given a nondegenerate Hermitian operator \hat{f} its real eigenvalues j are specified completely but its normalised eigenfunctions are determined only to within an arbitrary phase factor $e^{i\alpha_j}$ which may depend in any way on j .*

We saw in section 6.1 how given any basis x on S another basis y can be postulated with specified transformation functions $\Phi(x_i|y_j)$. These transformation functions can in turn be specified by declaring them to be the eigenfunctions of a linear Hermitian operator \hat{f} on functions of i (or rather eigenfunctions of a complete set of linear Hermitian operators represented symbolically by \hat{f} as described above). Therefore any supposed basis y (or basic property P_y) can be associated with a linear Hermitian operator \hat{f} . The real eigenvalues j associated with the eigenfunctions of \hat{f} serve to label the eigenfunctions so defined and to quantify the physical property P_y . This of course is to follow the procedure in the normal formulation of quantum mechanics. To make the transformation functions unique however, the j dependence of the indeterminate phase factor in them has to be specified†.

6.3 Observations concerning the law of inferred dynamical properties

First, generally speaking, suppose Y_j $j=1,\dots,N$ are pure states of knowledge in relation to a complete sample space S of order N . If the corresponding wave functions $\Phi(x_i|Y_j)$ over a basis x in S are orthogonal, i.e. if

$$\sum_{i=1}^N \Phi(x_i|Y_j)\Phi^*(x_i|Y_{j'}) = \delta_{jj'} \quad j, j' = 1, \dots, N. \quad (6.3.1)$$

* This limitation could perhaps be overcome by introducing another operator \hat{h} defined by $\hat{h}\Phi(y_j|x_i) = i\Phi(y_j|x_i)$ for all i and j . Then, given operators \hat{f} and \hat{h} , there is a basis y defined almost perfectly (i.e. to within a constant phase factor) as one for which the functions $\Phi(x_i|y_j)$ are eigenfunctions of \hat{f} with eigenvalues j and the functions $\Phi(y_j|x_i)$ (the conjugates of $\Phi(x_i|y_j)$) are eigenfunctions of \hat{h} with eigenvalues i .

† This is something of a sore point in the usual interpretation of quantum mechanics. The choice of the j dependence of the phase factor can appear arbitrary. In the present interpretation a definite j dependence of the phase of the transformation functions follows from postulated physical laws governing the basic properties (see for example the derivation of the position/position transformation functions in Chapter IV, the momentum/momentum transformation functions in Chapter VI or the spin/spin transformation functions in Chapters VIII and IX.)

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and if they form a complete set, then the alternative wave functions $\Phi(y_k|Y_j)$ over another basis y of S are also orthogonal and also form a complete set. The proof is as follows.

Proof of orthogonality of the $\Phi(y_k|Y_j)$

By Feynman's law

$$\sum_k \Phi(y_k|Y_j)\Phi^*(y_k|Y_{j'}) = \sum_k \sum_i \Phi(y_k|x_i)\Phi(x_i|Y_j)\sum_{i'} \Phi^*(y_k|x_{i'})\Phi^*(x_{i'}|Y_{j'})$$

where here and in the rest of this section all sums with unspecified limits run from 1 to N , and since the transformation functions $\Phi(y_k|x_i)$ are orthonormal the RHS reduces to

$$\sum_i \Phi(x_i|Y_j)\Phi^*(x_i|Y_{j'})$$

which by (6.3.1) is $\delta_{jj'}$. This shows the $\Phi(y_k|Y_j)$ are orthogonal.

Proof of completeness of the $\Phi(y_k|Y_j)$

By hypothesis, any wave function $\Phi(x_i|Y)$ can be written as

$$\Phi(x_i|Y) = \sum_{j=1}^N a_j \Phi(x_i|Y_j)$$

where the a_j are N complex constants. But by Feynman's law

$$\Phi(y_k|Y) = \sum_i \Phi(y_k|x_i)\Phi(x_i|Y) = \sum_i \sum_j \Phi(y_k|x_i)a_j\Phi(x_i|Y_j) = \sum_j a_j\Phi(y_k|Y_j)$$

showing the wave function $\Phi(y_k|Y)$ can be expanded in the $\Phi(y_k|Y_j)$ using the same constants a_j . Since $\Phi(x_i|Y)$ can be any wave function in the x representation, $\Phi(y_k|Y)$ can be any wave function in the y representation, so we have shown completeness of the wave functions $\Phi(y_k|Y_j)$.

Now with regard to the law of inferred dynamical properties (as formulated in section 3.12 of Chapter I) we note that knowledge of the possession of an inferred property P_j for any one value of j ($j=1,\dots,N$) can arise only when we hold pure knowledge Y_j or

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hold one or other of the pure states of knowledge Y'_j, Y''_j, \dots whose wave functions $\Phi(x_i|Y'_j), \Phi(x_i|Y''_j), \dots$ differ from $\Phi(x_i|Y_j)$ only with regard to their absolute phases. Accordingly we have for the wave functions $\Phi(x_i|P_j)$ ($j=1, \dots, N$) (where P_j stands for the proposition claiming property P_j applies) the formula

$$\Phi(x_i|P_j) = \Phi(x_i|Y_j)e^{i\alpha_j} \quad j=1, \dots, N \quad (6.3.2)$$

where the Y_j ($j=1, \dots, N$) are pure states of knowledge for which each wave function $\Phi(x_i|Y_j)$ ($j=1, \dots, N$) has a determinate or indeterminate absolute phase, and the α_j are indeterminate phases.

Now if the wave function $\Phi(x_i|Y)$ under any pure state of knowledge Y is expanded in terms of the set of N orthogonal wave functions $\Phi(x_i|Y_j)$ thus

$$\Phi(x_i|Y) = \sum_{j=1}^N a_j \Phi(x_i|Y_j) \quad (6.3.3)$$

where the a_j are N complex constants whose squared moduli must sum to 1 and whose values are (as we have seen) independent of the basis, then $|a_j|^2$ is our degree of belief (under knowledge Y) that property P is quantified by j .^{*} For we have, by Feynman's law (3.5.2) of Chapter I, that

$$\Phi(P_j|Y) = \sum_i \Phi(P_j|x_i)\Phi(x_i|Y)$$

^{*} To this result and to the (quantum mechanical) law of inferred dynamical properties there is a somewhat analogous (though much less fundamental or far reaching) law (or rather theorem) in classical mechanics using classical probability: if for example $\rho(\mathbf{r}, \mathbf{v})$ is our classical probability density in the 6-D μ -space representing dynamical states (position and velocity) of a single particle system, and if $\rho_j(\mathbf{r}, \mathbf{v})$

$j=1, \dots, N$ are a set of orthogonal probability densities (i.e. densities satisfying

$$\iint \rho_j(\mathbf{r}, \mathbf{v}) \rho_{j'}(\mathbf{r}, \mathbf{v}) d^3\mathbf{r} d^3\mathbf{v} = \delta_{jj'}) \text{ and if } \rho(\mathbf{r}, \mathbf{v}) \text{ is expressible as } \rho(\mathbf{r}, \mathbf{v}) = \sum_{j=1}^N a_j \rho_j(\mathbf{r}, \mathbf{v}), \text{ then to}$$

every such set $\rho_j(\mathbf{r}, \mathbf{v})$ of distributions there corresponds a property P of the particle quantified by j and a_j is the probability that P is quantified by j . The general form of the $\rho_j(\mathbf{r}, \mathbf{v})$ is $k_j \rho(\mathbf{r}, \mathbf{v})$ or 0 where k_j is a normalisation factor and zero applies when a certain function $f(\mathbf{r}, \mathbf{v})$ (representing a dynamical property) lies outside the range $f_j < f(\mathbf{r}, \mathbf{v}) < f_{j+1}$. For example $f(\mathbf{r}, \mathbf{v})$ might be

$f(\mathbf{r}, \mathbf{v}) = \frac{1}{2} m v^2$ (m being the particle mass) and then $f_j < f(\mathbf{r}, \mathbf{v}) < f_{j+1}$ represents the property that the kinetic energy of the particle lies in one of N ranges specified by j .

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where, by the general law of reciprocity ((3.11.1) of Chapter I), $\Phi(P_j|x_i) = \Phi^*(x_i|P_j)$. And by (6.3.2) and (6.3.3)

$$\Phi(P_j|Y) = \sum_i \sum_l \Phi^*(x_i|P_j) a_l \Phi(x_i|P_l) e^{-i\alpha_l} .$$

But since the $\Phi(x_i|P_j)$ are orthonormal this reduces to

$$\Phi(P_j|Y) = a_j e^{-i\alpha_j}$$

giving $|\Phi(P_j|Y)|^2 = |a_j|^2$ QED. And we note that we can formally rewrite (6.3.3) as

$$\Phi(x_i|Y) = \sum_{j=1}^N \Phi(P_j|Y) e^{i\alpha_j} \Phi(x_i|Y_j) = \sum_{j=1}^N \Phi(x_i|P_j) \Phi(P_j|Y) \quad (6.3.4)$$

which resembles Feynman's law (3.5.1) of Chapter I.

But we do not claim that the propositions P_j ($j=1, \dots, N$) (which the Y_j ($j=1, \dots, N$) respectively imply) necessarily form a *basis* in S . Nor do we generally claim at any specified time to be able (under knowledge Y) to get to know instantly by chance the value of the property variable j .

In the special case that the wave functions $\Phi(x_i|Y_j)$, $\Phi(x_i|Y'_j), \dots$ are (to within constant phase factors) the same as any of the transformation functions $\Phi(x_i|y_j)$, $\Phi(x_i|y'_j), \dots$ from one or other of a complete set* of equivalent correspondingly ordered bases y, y', \dots to basis x , then, by the law of inferred dynamical properties $P_j = y_j + y'_j + \dots$. Any one of the propositions P_j, y_j, y'_j, \dots then implies any other. In this case we can write (6.3.2) as

$$\Phi(x_i|P_j) = \Phi(x_i|y_j) e^{i\alpha_j} \quad j=1, \dots, N$$

where the α_j are indeterminate phases, and we have by Feynman's law and the general law of reciprocity that

$$\Phi(y_j|P_j) = \sum_{i=1}^N \Phi(y_j|x_i) \Phi(x_i|P_j) = \sum_{i=1}^N \Phi^*(x_i|y_j) \Phi(x_i|y_j) e^{i\alpha_j} = e^{i\alpha_j} .$$

* We include the case (if it should arise) where the basis y_j has no equivalent bases. And then of course $P_j = y_j$. (See last footnote to section 3.12 of Chapter I.)

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So, by the first law of extreme values of probability, and since we already know from our general knowledge G that P_j, y_j, y'_j, \dots imply one another, it must be that $P_j \stackrel{-\alpha_j}{\Leftrightarrow} \alpha_j y_j$ where the phases of implication α_j are indeterminate. Similarly we have $P_j \stackrel{-\alpha'_j}{\Leftrightarrow} \alpha'_j y'_j$ where the α'_j are indeterminate, and so on. So even though the $\alpha_j, \alpha'_j, \dots$ are indeterminate, these relations of implication must clearly apply and, as is always the case with implications, they apply regardless of any knowledge we may or may not hold of the dynamical properties of the quantum mechanical system under study.

Given any wave function $\Phi(x_i|Y)$ it is clear, from the very many wave functions possible, that we may well be able to construct $N-1$ other (mutually orthogonal) wave functions orthogonal to $\Phi(x_i|Y)$. By applying the law of inferred dynamical properties to all these N wave functions we see that *any* pure knowledge Y is (as far as knowledge of the system dynamics is concerned) equivalent to knowledge that a certain property of the system has a particular value.

If two sets of orthogonal wave functions $\Phi(x_i|Y_j)$ ($j=1, \dots, N$) and $\Phi(x_i|Y'_k)$ ($k=1, \dots, N$) share (to within a constant phase factor) a common wave function $\Phi(x_i|Y)$ so that for a certain j and a certain k

$$\Phi(x_i|Y_j)e^{i\alpha} = \Phi(x_i|Y'_k)e^{i\beta} = \Phi(x_i|Y) \quad (6.3.5)$$

where α and β are constant phases (independent of i), then, as regards knowledge of the dynamical properties of the system, knowledge Y is the same (pure) state of knowledge as Y_j or Y'_k and accordingly the same as knowledge that a certain property P of the system has value j or that a certain other property P' of the system has value k . Clearly there may in fact be very many ways in which a particular pure state of knowledge of system dynamics can be expressed in terms of the value of a possessed property. But we cannot generally claim, for example, that property P having value j implies property P' has value k independently of our knowledge.* We claim instead that *acquisition* of knowledge P'_k physically ensures the presence of property P_j . Expressed algebraically, Feynman's law and the general law of reciprocity gives

$$\Phi(P_j|P'_k) = \sum_i \Phi(P_j|x_i)\Phi(x_i|P'_k) = \sum_i \Phi^*(x_i|P_j)\Phi(x_i|P'_k)$$

where, on account of (6.3.2) and (6.3.5)

* To do so would open us up to the Kochen-Specker paradox (see section 1 of Chapter XV).

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$$\begin{aligned}\Phi(x_i|P_j) &= \Phi(x_i|Y_j)e^{i\alpha_j} = \Phi(x_i|Y)e^{-i\alpha}e^{i\alpha_j} \\ \Phi(x_i|P'_k) &= \Phi(x_i|Y'_k)e^{i\beta_k} = \Phi(x_i|Y)e^{-i\beta}e^{i\beta_k}\end{aligned}$$

where α_j and β_k are indeterminate phases unrelated to each other and to the phases α and β . Hence we arrive at

$$\Phi(P_j|P'_k) = e^{i(\alpha-\beta)}e^{i(\beta_k-\alpha_j)}$$

where the net phase $\alpha - \beta + \beta_k - \alpha_k$ is indeterminate. By the first law of extreme values of probability this result is consistent with what we claim to be the case – that *acquisition* of knowledge of the property P'_k physically ensures the presence of the property P_j .

It follows also from the law of inferred dynamical properties that if our sample space S refers to time period t_0 to t_1 and if $Y_j(t')$ ($j=1,\dots,N$) are pure states of knowledge formally functions of a parameter t' for $t_0 < t' < t_1$ and the corresponding wave functions $\Phi(x_i|Y_j(t'))$ over any basis x in S are orthogonal and form a complete set for any value t' between t_0 to t_1 , then to the pure states of knowledge $Y_j(t')$ ($j=1,\dots,N$) there corresponds a parameterised property $P(t')$ of the system S quantified by the variable j and associated with time t' in the time interval t_0 to t_1 . Or we may just as well say property $P(t')$ is ‘present at the time t' in that same time interval’. Thus associated with any aforementioned set $Y_j(t')$ ($j=1,\dots,N$) of pure states of knowledge parameterised by t' with $t_0 < t' < t_1$, we may claim there is a real dynamical property $P(t')$ possessed by S at time t' which varies with time t' ($t_0 < t' < t_1$) and takes possible values represented by j ($j=1,\dots,N$).

As far as our knowledge of system dynamics is concerned the propositions $Y_j(t')$ and $P_j(t')$ (where we let $P_j(t')$ stand for the proposition claiming property $P(t')$ is quantified by j) are the same, so that

$$\Phi(x_i|P_j(t')) = \Phi(x_i|Y_j(t'))e^{\alpha_j(t')} \quad (t_0 < t' < t_1) \quad (6.3.6)$$

as in (6.3.2), the $\alpha_j(t')$ being (for the various different values of j and t') indeterminate and unrelated.

Let a wave function $\Phi(x_i|Y)$ over a basis x in S be expanded in terms of the N orthogonal wave functions $\Phi(x_i|Y_j(t'))$ for any one value of the parameter t' . Then the coefficients a_j must of course be formally functions of t' so we will have

$$\Phi(x_i|Y) = \sum_{j=1}^N a_j(t') \Phi(x_i|Y_j(t')). \quad (6.3.7)$$

Now suppose x is a time-dependent basis*. Then with x_i replaced by $x_i(t)$ representing the same dynamical property of S at various times t , the LHS of (6.3.7) is a function of time t for $t_0 < t < t_1$. It is an evolving wave function $\Phi(x_i(t)|Y_j)$. Putting $t' = t$ we have the possible expansion

$$\Phi(x_i(t)|Y) = \sum_{j=1}^N a_j(t) \Phi(x_i(t)|Y_j(t)). \quad (6.3.8)$$

Using (6.3.6) in (6.3.8) we see that any time dependent wave function can be expanded thus:

$$\Phi(x_i(t)|Y) = \sum_{j=1}^N a_j(t) \Phi(x_i(t)|P_j(t)). \quad (6.3.9)$$

where the $a_j(t)$ differ from the $a_j(t)$ in (6.3.8) only with regard to their phases and $|a_j(t)|^2$ is our degree of belief under knowledge Y that property $P(t)$ is quantified by j . In practice, when employing (6.3.9) it is convenient to fix the j dependence of the absolute phases of the $\Phi(x_i(t)|P_j(t))$ in a conventional way (as is always done in ordinary quantum theory).†

6.4 Association of inferred properties with operators

By the law of inferred dynamical properties (section 3.12 of Chapter I) there is a property P associated with any one complete set of orthogonal wave functions $\Phi(x_i|Y_j)$ over a basis x_i . Pure knowledge Y_j is, as regards knowledge of system dynamics, the same as knowledge that P is quantified by j , i.e. that the system in question has property P_j .

* see fifth footnote to section 3.1 of Chapter I

† The important application of the law of inferred dynamical properties and the formula (6.3.9) arises in connection with the dynamical property represented, in the usual formalism of quantum mechanics, by the (generally time dependent) Hamiltonian operator for the system. Its eigenfunctions, which form a complete set, are an example of the $\Phi(x_i(t)|P_j(t))$ above where $P_j(t)$ then claims that the (non-basic) dynamical property called the ‘energy of the system at time t ’ is j or, in the case of degeneracy of the Hamiltonian operator, $P_j(t)$ claims particular values of a *number* of (separately non-basic) properties [such as the ‘energy’, ‘angular momentum’ and the ‘ z component of angular momentum at time t ’ in the case of a single particle in a (possibly time dependent) central field] all of which are needed to specify each eigenfunction of the complete set (see section 6.4).

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Taking one such complete set of orthogonal wave functions $\Phi(x_i|Y_j)$ that are not necessarily transformation functions, a linear operator \hat{f} on functions of i may always be defined by the equation

$$\hat{f} \Phi(x_i|Y_j) = j\Phi(x_i|Y_j)$$

holding for all the (real) parameter values j . Or more generally if j stands for M independent real parameters j_1, \dots, j_M needed to enumerate the propositions Y_j or to quantify the associated M dimensional property P_j then \hat{f} stands for a *set* of linear operators $\hat{f}_1, \dots, \hat{f}_M$ satisfying

$$\hat{f}_k \Phi(x_i|Y_j) = j_k \Phi(x_i|Y_j), \quad k = 1, \dots, M$$

simultaneously. Or if $j'_k = g_k(j_1, \dots, j_M)$, $k = 1, \dots, M$, is a 1-1 and real transformation then we have operators $\hat{f}'_k = g_k(\hat{f}_1, \dots, \hat{f}_M)$ for $k = 1, \dots, M$. However the parameters j_k are defined, the corresponding operators \hat{f}_k clearly commute with one another and form a complete set, meaning that any linear operator that commutes with the \hat{f}_k can only be a function of them.

It is therefore possible to associate with an inferred (not necessarily basic) property P of the quantum mechanical process, a definite linear Hermitian operator, or a complete commuting set of such operators. However the converse is not necessarily true. That is, we do not assume that to every complete set of commuting linear Hermitian operators there corresponds a property. This is only the case when the simultaneous eigenfunctions of those operators qualify as wave functions.

6.5 Pseudo bases, pseudo wave functions and pseudo transformation functions

An inferred property P_j ($j = 1, \dots, N$) in a sample space S of order N is not generally a basic property because the wave functions $\Phi(x_i|P_j)$ over any basis x do not generally satisfy a requirement of transformation functions, i.e. the $\Phi(x_i|P_j)$ are not specified to within a constant phase factor independent of i and j (see formula (6.3.2)). Nonetheless the probability distributions $\Phi(P_j|Y)$ under pure states of knowledge Y exhibit many of the same properties as wave functions. For this reason we call them ‘pseudo wave

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functions' and we say the propositions P_j ($j=1,\dots,N$) claiming the properties P_j ($j=1,\dots,N$) form a 'pseudo basis' in S .*

We have seen already that any wave function $\Phi(x_i|Y)$ can be expressed formally, using Feynman's law in the form (6.3.4), in terms of the pseudo wave functions $\Phi(P_j|Y)$ and the 'half-pseudo transformation functions' $\Phi(x_i|P_j)$. We also have by Feynman's law (3.5.2) of Chapter I that

$$\Phi(P_j|Y) = \sum_{i=1}^N \Phi(P_j|x_i)\Phi(x_i|Y) \quad (6.5.1)$$

and substituting for $\Phi(x_i|Y)$ in this law using the relation $\Phi(x_i|Y) = \sum_{k=1}^N \Phi(x_i|Q_k)\Phi(Q_k|Y)$, which is result (6.3.4) written for any inferred property Q_k different from P_j , we obtain

$$\Phi(P_j|Y) = \sum_{k=1}^N \Phi(P_j|Q_k)\Phi(Q_k|Y) \quad (6.5.2)$$

so a Feynman's law relation between pseudo wave functions is also formally valid using 'pseudo transformation functions' (the $\Phi(P_j|Q_k)$ in (6.5.2)).

It is also the case that the product rule for wave functions (section 3.7 of Chapter I) holds also for pseudo wave functions. So if $S^{(1)}, \dots, S^{(M)}$ are M closed sample spaces for systems $S^{(1)}, \dots, S^{(M)}$ respectively covering the same time period and we hold pure states of knowledge $Y^{(1)}, \dots, Y^{(M)}$ in each sample space, then with $P_j^{(1)}, \dots, P_l^{(M)}$ standing for inferred properties of the $S^{(1)}, \dots, S^{(M)}$ and $P_j^{(1)}, \dots, P_l^{(M)}$ for the propositions in $S^{(1)}, \dots, S^{(M)}$ respectively claiming those inferred properties, then

$$\Phi(P_j^{(1)} \dots P_l^{(M)} | Y^{(1)} \dots Y^{(M)}) = \Phi(P_j^{(1)} | Y^{(1)}) \dots \Phi(P_l^{(M)} | Y^{(M)}) \quad (6.5.3)$$

is always true.

We can prove (6.5.3) using the Feynman law relations

$$\Phi(P_j^{(n)} | Y^{(n)}) = \sum_i \Phi(P_j^{(n)} | x_i^{(n)}) \Phi(x_i^{(n)} | Y^{(n)}), \quad n = 1, \dots, M \quad (6.5.4)$$

* We stress that a pseudo wave function $\Phi(P_j|Y)$ does not completely specify the pure state of knowledge Y because the phases of the probabilities $\Phi(P_j|Y)$ are indeterminate and different for each value of j and no wave function can be calculated from knowledge of the moduli $|\Phi(P_j|Y)|$ alone.

and

$$\Phi(P_j^{(1)} \dots P_l^{(M)} | Y^{(1)} \dots Y^{(M)}) = \sum_{i, \dots, k} \Phi(P_j^{(1)} \dots P_l^{(M)} | x_i^{(1)} \dots x_k^{(M)}) \Phi(x_i^{(1)} \dots x_k^{(M)} | Y^{(1)} \dots Y^{(M)}) \dots (6.5.5)$$

where the $x_i^{(n)}$ ($n=1, \dots, M$) are contemporary bases in $S^{(1)}, \dots, S^{(M)}$ respectively and the sums are over all values of the indicated parameter(s). Putting $\Phi(x_i^{(1)} \dots x_k^{(M)} | Y^{(1)} \dots Y^{(M)}) = \Phi(x_i^{(1)} | Y^{(1)}) \dots \Phi(x_k^{(M)} | Y^{(M)})$ in (6.5.5) we find that (6.5.3) is equivalent to

$$\sum_{i, \dots, k} [\Phi(P_j^{(1)} \dots P_l^{(M)} | x_i^{(1)} \dots x_k^{(M)}) - \Phi(P_j^{(1)} | x_i^{(1)}) \dots \Phi(P_l^{(M)} | x_i^{(M)})] \Phi(x_i^{(1)} | Y^{(1)}) \dots \Phi(x_k^{(M)} | Y^{(M)}) = 0.$$

But this is evidently true because the conjugate of the expression inside the square brackets is zero on account of the general law of reciprocity and the ordinary product rule for wave functions QED.

Note that the pseudo bases $P_j^{(1)}, \dots, P_l^{(M)}$ in the product rule (6.5.3) for pseudo wave functions may refer to different times. Clearly the proof of (6.5.3) is independent of whether or not this is the case. When it is the case we can write the bases as $P_j^{(1)}(t_1), \dots, P_l^{(M)}(t_M)$ where t_1, \dots, t_M are the times to which they refer. The general pseudo basis $P_j^{(1)}(t_1) \dots P_l^{(M)}(t_M)$ in the combined sample space $S = S^{(1)} \dots S^{(M)}$ is a pseudo basis not referring to a single time.

We note also that the proof of (6.5.3) works just as well with the pseudo bases changed to time-dependent *proper* bases $y_j^{(1)}, \dots, y_l^{(M)}$. There is therefore the possibility of starting with proper bases $y_j^{(1)}(t_1), \dots, y_l^{(M)}(t_M)$ in certain closed sample spaces $S^{(1)}, \dots, S^{(M)}$ (where $y_j^{(1)}(t_1)$ refers to time t_1 in $S^{(1)}$, $y_k^{(2)}(t_2)$ refers to time t_2 in $S^{(2)}$, ...etc) and constructing a new kind of basis $y_j^{(1)}(t_1) \dots y_l^{(M)}(t_M)$ in S which does not refer to a single time. The product rule for wave functions then generalises to include these new kinds of bases. And if $\Phi(y_j^{(1)}(t_1) | Y^{(1)}), \dots, \Phi(y_l^{(M)}(t_M) | Y^{(M)})$ are wave functions in the separate sample spaces we have a new kind of wave function in S (under knowledge $Y^{(1)} \dots Y^{(M)}$) which is the product of the wave functions $\Phi(y_j^{(1)}(t_1) | Y^{(1)}), \dots, \Phi(y_l^{(M)}(t_M) | Y^{(M)})$ in the separate sample spaces.

However we will not find a need to employ bases and wave functions of this new kind in the present monograph (whether the bases from which they are derived are proper bases or pseudo bases). So pseudo bases of the form $P_j^{(1)} \dots P_l^{(M)}$ in the combined sample space $S = S^{(1)} \dots S^{(M)}$ will always be taken to refer to a single time, i.e. the pseudo bases $P_j^{(1)}, \dots, P_l^{(M)}$ will be always contemporary. And proper bases of the form $y_j^{(1)} \dots y_l^{(M)}$ in the

combined sample space $S = S^{(1)} \dots S^{(M)}$ will always be made up from contemporary proper bases $y_j^{(1)}, \dots, y_l^{(M)}$ in $S^{(1)}, \dots, S^{(M)}$ respectively.

7. Law of partial orthonormal decomposition

7.1 Statement of the Law

Suppose $S^{(1)}$ and $S^{(2)}$ are contemporary and closed sample spaces of order $N^{(1)}$ and $N^{(2)}$ respectively. And suppose $x_i^{(1)}$ and $x_j^{(2)}$ are bases in $S^{(1)}$ and $S^{(2)}$ respectively pertaining to the same time t . And suppose also that $x_j^{(2)}$ is a *primary* basis in $S^{(2)}$. Using basis $x_i^{(1)} x_j^{(2)}$ in $S^{(1)} S^{(2)}$ let our knowledge Y (represented by a wave function $\Phi(x_i^{(1)} x_j^{(2)} | Y)$) be pure but *inseparable* (not expressible as pure knowledge in relation to $S^{(1)}$ and $S^{(2)}$ separately). Now we may take the transformation functions $\Phi(x_i^{(1)} | y_k^{(1)})$ in $S^{(1)}$ where $y_k^{(1)}$ is a *primary* basis in $S^{(1)}$ (different from the basis $x_i^{(1)}$ but pertaining to the same time t), and expand the wave function $\Phi(x_i^{(1)} x_j^{(2)} | Y)$ in the complete set of functions $\Phi(x_i^{(1)} | y_k^{(1)})$ of $x_i^{(1)}$. That is we can write

$$\Phi(x_i^{(1)} x_j^{(2)} | Y) = \sum_k a_k h_{kj} \Phi(x_i^{(1)} | y_k^{(1)}) \quad (7.1.1)$$

where k runs from 1 to $N^{(1)}$, the a_k are positive or zero and the h_{kj} are suitable normalised functions of j :

$$\sum_j |h_{kj}|^2 = 1 \quad \text{for all } k \quad (7.1.2)$$

where j runs from 1 to $N^{(2)}$. The a_k are necessary constants, the sum of their squares being equal to 1 for normalisation of $\Phi(x_i^{(1)} x_j^{(2)} | Y)$ in (7.1.1)).*

Then, according to the law of partial orthonormal decomposition, $|a_k|^2$ ($k = 1, \dots, N^{(1)}$) is our degree of belief distribution over the $y_k^{(1)}$, i.e.

$$|a_k|^2 = |\Phi(y_k^{(1)} | Y)|^2. \quad (7.1.3)$$

* If $a_k h_{kj}$ has to be zero for a certain value of k in the expansion (7.1.1) then we make $a_k = 0$ for that k and h_{kj} (for that k) may be any normalised function of j we please.

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And the h_{kj} ($j=1,\dots,N^{(2)}$) are, to within constant (i.e. only k dependent) phase factors, our probability distributions over the $x_j^{(2)}$ on learning the truth of $y_k^{(1)}$, that is

$$\Phi(x_j^{(2)}|y_k^{(1)}Y) = h_{kj}e^{i\varepsilon_k} \quad (7.1.4)$$

where the ε_k are indeterminate constant phases for each value of k . Our knowledge $y_k^{(1)}Y$ is then separable into knowledge $Y^{(1)}$ pure in relation to $S^{(1)}$ and knowledge $Y^{(2)}$ pure in relation to $S^{(2)}$.

7.2 Proof of the law

Since $y_k^{(1)} \rightarrow \sum_{j=1}^{N^{(2)}} (y_k^{(1)}x_j^{(2)})$ (where summation signifies disjunction), learning the truth of $y_k^{(1)}$ would each time be a case of harmless conditioning over the primary basis $y_i^{(1)}x_j^{(2)}$ in $S^{(1)}S^{(2)}$ (see section 3.6 of Chapter I). After such harmless conditioning our wave function over basis $y_i^{(1)}x_j^{(2)}$ in $S^{(1)}S^{(2)}$ can, by (4.2), be written

$$\Phi(y_i^{(1)}x_j^{(2)}|y_k^{(1)}Y) = \delta_{ik} \frac{\Phi(y_i^{(1)}x_j^{(2)}|Y)e^{-i\kappa}}{\Phi(y_k^{(1)}|Y)} \quad (7.2.1)$$

where κ is the phase characteristic of knowledge Y . Here we can replace $y_i^{(1)}$ on the RHS by $y_k^{(1)}$ and we see that the RHS is (for any k) a product of a function of i and a function of j . Knowledge $y_k^{(1)}Y$ is therefore separable into pure knowledge $Y^{(1)}$ in $S^{(1)}$ and pure knowledge $Y^{(2)}$ in $S^{(2)}$. And we have accordingly wave functions

$$\begin{aligned} \Phi(y_i^{(1)}|y_k^{(1)}Y) &= \delta_{ik}e^{i\gamma_k} \\ \Phi(x_j^{(2)}|y_k^{(1)}Y) &= \frac{\Phi(y_k^{(1)}x_j^{(2)}|Y)e^{-i\kappa}}{\Phi(y_k^{(1)}|Y)}e^{-i\gamma_k} \end{aligned} \quad (7.2.2)$$

where κ and γ_k are indeterminate constant phases.

Now by Feynman's law in the special form (5.2) our original wave function $\Phi(x_i^{(1)}x_j^{(2)}|Y)$ can be expanded thus

$$\Phi(x_i^{(1)}x_j^{(2)}|Y) = \sum_k \Phi(x_i^{(1)}|y_k^{(1)})\Phi(y_k^{(1)}x_j^{(2)}|Y). \quad (7.2.3)$$

Comparing this with (7.1.1) we see (using the second of (7.2.2)) that

$$a_k h_{kj} = \Phi(y_k^{(1)} x_j^{(2)} | Y) = \Phi(y_k^{(1)} | Y) \Phi(x_j^{(2)} | y_k^{(1)} Y) e^{i\kappa} e^{i\gamma_k} \quad (7.2.4)$$

If, for some k , $a_k = 0$ then by (7.2.4) $\Phi(y_k^{(1)} | Y) = 0$ (since $\Phi(x_j^{(2)} | y_k^{(1)} Y)$ cannot be zero for all j). This proves (7.1.3) in the case $a_k = 0$. Also, when $a_k = 0$ we are free to choose the indeterminate h_{kj} as we please.* Since $\Phi(y_k^{(1)} | Y) = 0$ also, we cannot learn the truth of $y_k^{(1)}$ so that $\Phi(x_j^{(2)} | y_k^{(1)} Y)$ is indeterminate. But we can choose h_{kj} to equal the indeterminate $\Phi(x_j^{(2)} | y_k^{(1)} Y) e^{-i\epsilon_k}$ and hence ensure the formal truth of (7.1.4) in the case $a_k = 0$.

If $a_k \neq 0$ then by (7.2.4)

$$h_{kj} = \frac{\Phi(y_k^{(1)} | Y)}{a_k} \Phi(x_j^{(2)} | y_k^{(1)} Y) e^{i\kappa} e^{i\gamma_k} \quad (7.2.5)$$

and since h_{kj} and $\Phi(x_j^{(2)} | y_k^{(1)} Y)$ are both normalised over j , (7.2.5) gives

$$\left| \frac{\Phi(y_k^{(1)} | Y)}{a_k} \right|^2 = 1 \quad (7.2.6)$$

which proves (7.1.3) when $a_k \neq 0$ and converts (7.2.5) to (7.1.4) QED.

8. A case of mixed knowledge

Suppose, as in section 7.1, that $S^{(1)}$ and $S^{(2)}$ are contemporary and closed sample spaces, and suppose $x_i^{(1)}$ and $x_j^{(2)}$ are bases in $S^{(1)}$ and $S^{(2)}$ respectively pertaining to the same time t . And suppose again that $x_j^{(2)}$ is a *primary* basis in $S^{(2)}$. Using basis $x_i^{(1)} x_j^{(2)}$ in $S^{(1)} S^{(2)}$, let our wave function, under knowledge Y pure and inseparable in relation to $S^{(1)} S^{(2)}$, be $\Phi(x_i^{(1)} x_j^{(2)} | Y)$. Then given a primary basis $y_k^{(1)}$ pertaining to time t in $S^{(1)}$ the law of partial orthonormal decomposition of section 7.1 applies.

Using the expansion (7.1.1), we have by the orthogonality of the $\Phi(x_i^{(1)} | y_k^{(1)})$ that

$$\sum_i \left| \Phi(x_i^{(1)} x_j^{(2)} | Y) \right|^2 = \sum_k \left| a_k h_{kj} \right|^2 \quad (8.1)$$

* See the footnote to section 7.1

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and with $y_k^{(1)}$ a primary basis in $S^{(1)}$, the result (7.2.4) means the RHS of (8.1) is $\sum_k |\Phi(y_k^{(1)}|Y)\Phi(x_j^{(2)}|y_k^{(1)}Y)|^2$ and by the sum rule we have for our probability distribution over the $x_j^{(2)}$ the formula

$$\Phi(x_j^{(2)}|Y) = \sqrt{\sum_i |\Phi(x_i^{(1)}x_j^{(2)}|Y)|^2} e^{i\alpha_j} = \sqrt{\sum_k |\Phi(y_k^{(1)}|Y)\Phi(x_j^{(2)}|y_k^{(1)}Y)|^2} e^{i\alpha_j} \quad (8.2)$$

where the α_j are indeterminate phases.

The probability distribution (8.2) cannot represent a pure state of knowledge because its relative phases are indeterminate. We say instead that it represents a state of knowledge ‘mixed’ in relation to $S^{(2)}$.*

If we should get to learn (by harmlessly conditioning) which of the $y_k^{(1)}$ was true then we should of course change our probability distribution from that in (8.2) to that given by (7.1.4) where the h_{kj} are determined by (7.1.1). This distribution *does* have determinate relative phases and therefore represents a state of knowledge pure in relation to $S^{(2)}$.

We see here the possibility of passing from a state of mixed knowledge in relation to $S^{(2)}$ to a state of pure knowledge in relation to $S^{(2)}$ having gained information in $S^{(1)}$.

Before such a transformation into pure knowledge the mixed knowledge can evidently be represented in different ways according to which primary basis $y_k^{(1)}$ is chosen in $S^{(1)}$. This choice is up to us and cannot possibly affect our probabilities of propositions in $S^{(2)}$. For each possible choice of this basis there will be different functions $\Phi(x_j^{(2)}|y_k^{(1)}Y)$. Let us say $y_k^{(1)}$ will give $\Phi(x_j^{(2)}|y_k^{(1)}Y)$, $y_k'^{(1)}$ will give $\Phi(x_j^{(2)}|y_k'^{(1)}Y)$, ...etc., $y_k^{(1)}$, $y_k'^{(1)}$, ...etc representing different primary bases in $S^{(1)}$.[†] From (8.2) we have in each case a prior probability distribution over $x_j^{(2)}$:

* ‘Mixed states’ of knowledge (as they are called) can occur in many other situations, and the general theory of mixed states of knowledge will be given in Chapter XIV. Note that on taking the modulus squared of both sides of (8.2) we get a result (for the squared moduli) the same as the relation we would expect between classical probabilities.

[†] The wave functions $\Phi(x_j^{(2)}|y_k^{(1)}Y)$, $\Phi(x_j^{(2)}|y_k'^{(1)}Y)$, ...etc. are different, so we can gain different pure states of knowledge in relation to $S^{(2)}$ depending on which of the properties (P_y or $P_{y'}$... etc) associated with $S^{(1)}$ we choose to measure. In the usual interpretation of quantum mechanics, that regards the wave function as the physical state of the system, this implies the possibility of controlling the physical state of a distant system (associated with $S^{(2)}$) by our choice of measurement on a nearby system (associated with $S^{(1)}$). But this strange action at a distance is not implied in the present interpretation where a different choice of measurement on the nearby system leads only (and quite naturally) to a different state of *knowledge* of the distant system.

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$$\Phi(x_j^{(2)}|Y) = \sqrt{\sum_k |\Phi(y_k^{(1)}|Y)\Phi(x_j^{(2)}|y_k^{(1)}Y)|^2} e^{i\alpha_j},$$

$$\Phi'(x_j^{(2)}|Y) = \sqrt{\sum_k |\Phi(y_k^{(1)}|Y)\Phi(x_j^{(2)}|y_k^{(1)}Y)|^2} e^{i\alpha'_j},$$

...etc.

These probability distributions must, by the uniqueness of probabilities, be the same. The moduli of them are necessarily equal as follows from the equalities

$$\begin{aligned} |\Phi(x_j^{(2)}|Y)|^2 &= \sum_k |\Phi(y_k^{(1)}|Y)\Phi(x_j^{(2)}|y_k^{(1)}Y)|^2 \\ &= \sum_k |\Phi(y_k^{(1)}|Y)\Phi(x_j^{(2)}|y_k^{(1)}Y)|^2 \\ &= \dots \text{etc.} \end{aligned} \tag{8.3}$$

which are a consequence of (8.1) and (7.2.4). And, for consistency, the phases $\alpha_j, \alpha'_j, \dots$, though indeterminate functions of j , must be the *same* indeterminate function of j , i.e.

$$\alpha_j = \alpha'_j = \alpha''_j = \dots$$

for each value of j .

9. Probability and expected frequencies

An important part of probability theory is the prediction of expected frequencies of occurrence of the possible outcomes in repeated trials of a process involving a system initially prepared in a certain way, or in simultaneous trials of processes involving identical systems similarly prepared and taking place together in different locations in space without interfering with one another.

Let S be a sample space of propositions about any one of the processes. And suppose S includes propositions X_i claiming occurrence of the i^{th} outcome out of n mutually exclusive and exhaustive possible outcomes of the process.* Our original (not necessarily pure) knowledge Y relating to S will be the same for any one of the processes.

Suppose $\Phi(X_i|Y)$ ($i = 1, \dots, n$) is our (complex-valued) probability distribution over the X_i (with determinate or indeterminate relative phases). Then, in a large number

* For example, if a large region R of space is divided up into n small volume elements dV_i ($i = 1, \dots, n$), X_i might claim that a particle (whose motion is initially prepared in a certain way so as to finish up somewhere in R) will in fact finish up in volume element dV_i .

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M of similar processes, the expected relative frequency f_i of cases in which X_i is true is given *under a certain condition* by the frequency rule

$$f_i = |\Phi(X_i|Y)|^2. \quad (9.1)$$

This follows from the ‘law of large numbers’ which can be proved from the general laws of complex-valued probability in much the same way as it is proved from the laws of classical probability. Although the classical proof is well known the proof in the new probability theory will be spelt out here because of its importance in the Bayesian approach to probability and because of the involvement of the law of absolute logical independence under pure knowledge in the case when Y is a pure state of knowledge and the separate sample spaces S for each member of the ensemble (of the contemporary or non-contemporary processes) are closed.

It will be sufficient to show that X_1 is expected to be true with relative frequency $|\Phi(X_1|Y)|^2$. This can be done by setting up sample spaces $S^{(1)}, \dots, S^{(M)}$ (which are the sample spaces S for each process) and their combination S^M that will include propositions which are the n^M conjunctions of the sort $X_i^{(1)} X_j^{(2)} \dots X_l^{(M)}$ any one of which claims X_i is true in the first process, X_j is true in the second process, ... X_l is true in the M^{th} process. Our knowledge relating to this sample space (the combination of the M sample spaces S) will be denoted Y^M . We will show that given certain knowledge Z is part of our general knowledge, the modulus squared of the probability of X_1^m where X_1^m is the proposition ‘ X_1 is true m times in the M processes’ has the binomial distribution in m , i.e.

$$|\Phi(X_1^m|Y^M)|^2 = {}_M C_m p^m (1-p)^{M-m} \quad (9.2)$$

where $p = |\Phi(X_1|Y)|^2$ and $1-p = |\Phi(\bar{X}_1|Y)|^2$. As is well known, the binomial distribution has a mean value $\bar{m} = Mp$ and a standard deviation $\sigma = \sqrt{Mp(1-p)}$ so that as $M \rightarrow \infty$ the ratio $\sigma/\bar{m} \rightarrow 0$ and the probability that m/M is inside the range $p - \delta p$ to $p + \delta p$ tends to one for any δp however small. That is, for large enough M the frequency rule (9.1) (with $i=1$) follows from (9.2).

We can prove (9.2) under the condition that the sample spaces $S^{(1)}, \dots, S^{(M)}$ are known to be logically independent of each other under knowledge Y^M . This is the required knowledge labelled Z above. And under knowledge Z , if it is possible to acquire knowledge of the outcomes of some of the processes as they occur* this knowledge is redundant in as far as it does not change our degree of belief in any

* We assume of course that acquisition of such knowledge could be achieved harmlessly with regard to the outcomes themselves and that knowledge of the outcomes would be compatible with knowledge Y^M .

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particular outcome of the other processes (see section 1.3). In the case when Y is a pure state of knowledge and the sample spaces $S^{(1)}, \dots, S^{(M)}$ are closed, the required logical independence is *necessarily* present because of the law of absolute logical independence under pure knowledge (section 3.7 Chapter I). In the case when Y is not a pure state of knowledge it is necessary to justify logical independence in some other way*; the difficulty in doing this with complete confidence gives credence to the idea, often expressed, that probabilities deduced under pure states of knowledge in quantum mechanics are more fundamental and more reliable than probabilities deduced under the non-pure states of knowledge in classical mechanics.

The proof of (9.2) can now be illustrated by example. Let $M=5$ and $m=3$ i.e. consider the probability that X_1 is true 3 times out of the 5. The probability for getting the sequence $X_1^{(1)} X_1^{(2)} \bar{X}_1^{(3)} \bar{X}_1^{(4)} X_1^{(5)}$ (which means, reading from left to right, that X_1 is true in the first process, true in the second, false in the third, ... etc.) is, by the specialised product rule (2.1),

$$\begin{aligned} & \Phi(X_1^{(1)} X_1^{(2)} \bar{X}_1^{(3)} \bar{X}_1^{(4)} X_1^{(5)} | Y^5) \\ &= \Phi(X_1^{(1)} | Y^5) \Phi(X_1^{(2)} | Y^5) \Phi(\bar{X}_1^{(3)} | Y^5) \Phi(\bar{X}_1^{(4)} | Y^5) \Phi(X_1^{(5)} | Y^5) e^{i4k} \end{aligned} \quad (9.3)$$

where k is the phase characteristic of knowledge Y^5 . So because, for example $\Phi(X_1^{(2)} | Y^5)$ and $\Phi(X_1 | Y)$ differ only with respect to their phases, we have

$$\left| \Phi(X_1^{(1)} X_1^{(2)} \bar{X}_1^{(3)} \bar{X}_1^{(4)} X_1^{(5)} | Y^5) \right| = \left| \Phi(X_1 | Y) \right|^3 \left| \Phi(\bar{X}_1 | Y) \right|^{5-3} \quad (9.4)$$

The number of possible sequences which claim X_1 is true in just 3 of the 5 processes is ${}_5C_3$. These sequences represent mutually exclusive propositions in the sample space S^M and their disjunction is X_1^m with $m=3$. Using the sum rule ((2.3.2) of Chapter I) we therefore have from (9.4) that

$$\left| \Phi(X_1^3 | Y^5) \right| = \sqrt{{}_5C_3 \left| \Phi(X_1^{(1)} X_1^{(2)} \bar{X}_1^{(3)} \bar{X}_1^{(4)} X_1^{(5)} | Y^5) \right|^2} = \sqrt{{}_5C_3 \left(\left| \Phi(X_1 | Y) \right|^2 \right)^3 \left(\left| \Phi(\bar{X}_1 | Y) \right|^2 \right)^{5-3}}$$

or

$$\left| \Phi(X_1^3 | Y^5) \right|^2 = {}_5C_3 p^3 (1-p)^{5-3} \quad (9.5)$$

* Of course cognitive and causal independence of the sample spaces (which we do assume) does not imply logical independence of them, and without being sure of logical independence, knowledge of the outcomes of some of the processes of the ensemble might well lead us to recalculate our probabilities for outcomes of the others (as for example in repeatedly rolling a die which might be biased).

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where $p = |\Phi(X_1|Y)|^2$. Clearly (9.5) generalises to (9.2) which holds for any values of M and m .

It follows from (9.2) that for large enough M , X_1 is (under knowledge Y^M and our general knowledge that includes Z) expected to be true with relative frequency close to $|\Phi(X_1|Y)|^2$ and similarly, for any i , that X_i is expected to be true with relative frequency close to f_i as given by (9.1).^{*} And this applies even when we could not in principle get to know which outcome occurs on each occasion.[†]

That X_i is, for large M , expected to be true with frequency $|\Phi(X_i|Y)|^2$ has been proved by calculating the probability (call it ϕ) that this is so and finding that ϕ has modulus 1 (in the limit $M \rightarrow \infty$). But because of the repeated use of the sum rule to do this, the phase $\angle\phi$ is generally indeterminate and we are unable for certain to claim that the relative frequency is determined *physically* (i.e. implied by knowledge Y^M or brought about by acquisition of that knowledge). And we insist that we would in fact generally be wrong in making that claim. Things would be different if $\angle\phi$ turned out to be *determinate*, but this is hardly ever the case.[‡]

As a corollary to the derivation of (9.1), it is noted that the expected relative frequency f_A of cases in which any disjunction A of the X_i is true is simply

$$f_A = \sum_i |\Phi(X_i|Y)|^2 = |\Phi(A|Y)|^2 \quad (9.6)$$

where the sum is over all the X_i in the disjunction A .

As a second corollary, we note that the mean value $\overline{x(i)}$ (in M trials) of any function $x(i)$ of i is (for large M) expected to be close to the ‘expected value’ defined by

^{*} Of course expected frequencies are generally not the same as actual frequencies. The former generally change with our knowledge while the latter do not. (See Appendix F for further discussion of this point.)

[†] If, for example, the X_i are the propositions of an improper basis (see section 1 of Chapter X) we could never get to know which of the X_i was true.

[‡] Even if the X_i form a basis in S , n equals the order N of S and Y is a pure state of knowledge with $\Phi(X_i|Y) = |\Phi(X_i|Y)|e^{i\alpha}$ where α is a known phase independent of i so the sum rule for wave functions might be employed in S^M , the phase $\angle\phi$ is still generally indeterminate. This is because, for $N \neq 2$, $X_1^{(1)} X_1^{(2)} \overline{X_1^{(3)}} \overline{X_1^{(4)}} X_1^{(5)}$ in (9.3) can only be expressed as a disjunction of the $X_1^{(1)} X_1^{(2)} \overline{X_i^{(3)}} \overline{X_j^{(4)}} X_1^{(5)}$ through use of the distribution rule (7th of (2.2.1.5) of Chapter I) which carries an indeterminate phase of implication. With $N = 2$ we *do* get a determinate $\angle\phi$ and this rather special case is the only one in which frequencies of outcomes are apparently determined physically.

$$E(x(i)) = \sum_{i=1}^n x(i) |\Phi(X_i|Y)|^2. \quad (9.7)$$

For the relative the frequency \tilde{f}_i at which the value i occurs in the M trials is expected to be close to $|\Phi(X_i|Y)|^2$. So replacing $|\Phi(X_i|Y)|^2$ by \tilde{f}_i , the RHS of (9.7) might be rewritten

$$\sum_{i=1}^n x(i) \tilde{f}_i \quad (9.8)$$

which is the sample mean value $\overline{x(i)}$. We therefore expect (for large M) that

$$\overline{x(i)} = E(x(i)). \quad (9.9)$$

10. Reasoning with certainty in quantum mechanics

The laws of extreme values of probability (section 2.2.2 of Chapter I) can sometimes be used to demonstrate an implied relation (between physical events) that exists quite independently of any knowledge we may or may not have of the dynamical properties of the quantum mechanical system in question.

If we start out with general knowledge G and if for example we can show, using the (complex-valued) probability calculus, that under supposed pure knowledge Y of the dynamical properties of a system

$$\Phi(X|Y) = e^{i\alpha}$$

where α is a real number with a definite (determinate) value, then by the first law of extreme values we can say

$$Y \Rightarrow^\alpha X.$$

This means that the dynamical property or event claimed by Y implies (with phase of implication α) the dynamical property or event claimed by X . So the one event must cause or imply the other as a consequence of the laws of motion, the unchanging properties of the system and the external fields present, all of which are known to us under the heading of our general knowledge G . (If in addition we can prove that $\Phi(Y|X) = e^{i\beta}$ where β is a determinate real number (which must in fact always equal $-\alpha$) then $X \Rightarrow^\beta Y$ also and we have demonstrated a *correlation* between X and Y .)

Being a consequence of the laws of motion, the unchanging properties of the system and the external fields, such an implied relation (or correlation) must apply

regardless of any knowledge we may or may not hold of the dynamical properties of the system in question.

10.1 Equivalent bases in a closed sample space

If x_i $i=1,\dots,N$ is a basis in a closed sample space S of order N then under certain pure states of knowledge we are certain which value of i applies. Each such state of knowledge involves of course knowledge of the truth of x_i for some value $i=k$. And by the laws of extreme values of probability our wave function in the x representation can be written as $\Phi(x_i|x_k)$ given by

$$\Phi(x_i|x_k) = \delta_{ik} \quad (10.1.1)$$

because $x_k \Rightarrow x_i|_{i=k}$ and $x_k \Rightarrow \bar{x}_i|_{i \neq k}$.

Now it can be that for a certain other basis y_j ($j=1,\dots,N$) in S (possibly referring to a property at a different time) the transfer functions from y to x take the form

$$\Phi(x_i|y_j) = \begin{cases} e^{i\alpha_j} & i = k_j \\ 0 & i \neq k_j \end{cases} \quad (10.1.2)$$

where the α_j are determinate phases and k_j is a generally different (known) integer in the range $1,\dots,N$ for each value ($j=1,\dots,N$) of j . In the matrix notation we might for example have

$$\Phi(x_i|y_j) = \begin{pmatrix} 0 & e^{i\alpha_2} & 0 & 0 & \dots \\ 0 & 0 & e^{i\alpha_3} & 0 & \\ e^{i\alpha_1} & 0 & 0 & 0 & \\ 0 & 0 & 0 & & \\ \vdots & & & & \end{pmatrix} \quad (10.1.3)$$

where every row and every column necessarily contains only one non-zero entry. This may apply also to certain other bases z_j $j=1,\dots,N$, ...etc so that $\Phi(x_i|y_j)$, $\Phi(x_i|z_j)$, $\Phi(z_i|y_j), \dots$ are all of the form (10.1.2) with generally different known functions k_j of j and generally different (but determinate) values α_j in each case. A *set* of bases of this

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kind will be called a ‘set of equivalent bases’ and we shall say any one of the bases of the set is ‘equivalent’ to any other.*

In relation to a set of equivalent bases x, y, z, \dots and under knowledge of the transformation functions between them we can reason with certainty using Feynman’s law to deduce the phases of implication.

First, given (10.1.2) we clearly have

$$\begin{cases} y_j \Rightarrow^{\alpha_j} x_i & i = k_j \\ y_j \Rightarrow \bar{x}_i & i \neq k_j \end{cases} \quad (10.1.4)$$

Second, because the inverse transfer function $\Phi(y_j|x_i)$ is the conjugate of $\Phi(x_i|y_j)$ we have also that

$$\begin{cases} x_i \Rightarrow^{-\alpha_j} y_j & i = k_j \\ x_i \Rightarrow \bar{y}_j & i \neq k_j \end{cases} \quad (10.1.5)$$

Hence propositions x_i and y_j (with $i = k_j$) are equivalent or

$$y_j \stackrel{-\alpha_j}{\Leftrightarrow} x_i \quad \text{when } i = k_j. \quad (10.1.6)$$

In the case that bases x and y are the same except perhaps for the order of their propositions[†] we must have full equivalence of corresponding propositions, i.e. $\alpha_j = 0$ in (10.1.6), since any proposition implies itself with phase of implication equal to zero.)

Third, by applying Feynman’s law to equivalent bases x, y and z (possibly referring to properties occurring at different times) we have

$$\Phi(y_j|z_m) = \sum_i \Phi(y_j|x_i)\Phi(x_i|z_m) \quad (10.1.7)$$

where, as well as (10.1.4) and (10.1.5),

$$\Phi(x_i|z_m) = \begin{cases} e^{i\beta_m} & i = l_m \\ 0 & i \neq l_m \end{cases}$$

* If the matrix in (10.3.1) is diagonal we say the bases x and y are ‘correspondingly ordered’ (as we did in section 3.10 of Chapter I). The matrix (4.4) in Chapter VII representing the spin/spin transfer function for the z components of spin in two coordinate systems sharing a common z axis is an example of a case in which the matrix representing a transformation function between equivalent bases is diagonal.

† In such a case the *natural* order of the propositions of x (or of y) remains the same but the order in which the propositions of x (or of y , or of both) are numbered may be different from the natural order.

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Clearly, for any given m , the summand in (10.1.7) is non-zero only for one value of i i.e. for $i = l_m$. Thus $\Phi(y_j|z_m)$ is zero except when j makes k_j equal to l_m and

$$\Phi(y_j|z_m) = \begin{cases} e^{i(\beta_m - \alpha_j)} & k_j = l_m \\ 0 & k_j \neq l_m \end{cases} \quad (10.1.8)$$

from which we deduce that

$$z_m^{-(\beta_m - \alpha_j)} \Leftrightarrow^{\beta_m - \alpha_j} y_j \quad \text{when } k_j = l_m. \quad (10.1.9)$$

Therefore, in reasoning with certainty over equivalent bases x, y and z in a closed sample space we have the following laws for phases of implication. Given any values of i, j and m :

$$\text{if } x_i \Rightarrow^\alpha y_j \text{ then } y_j \Rightarrow^{-\alpha} x_i \quad (10.1.10)$$

and

$$\text{if } x_i \Rightarrow^\alpha y_j \text{ and } y_j \Rightarrow^\beta z_m \text{ then } x_i \Rightarrow^{\alpha+\beta} z_m. \quad (10.1.11)$$

Note that (10.1.11) is in agreement with (or provided the original reason for claiming) the general rule of phase addition in (2.2.1.2) of Chapter I.

10.2 Changes in the phases of wave functions under reasoning with certainty

Let x, y and z be bases of a closed sample space and suppose only y and z are equivalent. Then our wave function $\Phi(x_i|y_j)$ generally has, for any i , a modulus less than 1 and we are uncertain as to which proposition x_i ($i = 1, \dots, N$) is true. Since y and z are equivalent $\Phi(y_j|z_m)$ is of the form (10.1.2) and by Feynman's law

$$\Phi(x_i|z_m) = \sum_j \Phi(x_i|y_j) \Phi(y_j|z_m). \quad (10.2.1)$$

On putting

$$\Phi(y_j|z_m) = \begin{cases} e^{i\alpha_m} & j = k_m \\ 0 & j \neq k_m \end{cases} \quad (10.2.2)$$

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we arrive at the rule:

$$\text{If } z_m^{-\alpha_m} \Leftrightarrow^{\alpha_m} y_j \text{ then } \Phi(x_i|z_m) = \Phi(x_i|y_j)e^{i\alpha_m} \quad (10.2.3)$$

If, instead of y and z , x and z are equivalent bases and Y any pure state of knowledge we can again use Feynman's law to derive the following rule (in which m and i are supposed to be related by the 1-1 relation $m = l_i$):

$$\text{If } x_i^{-\alpha_m} \Leftrightarrow^{\alpha_m} z_m \text{ then } \Phi(x_i|Y) = \Phi(z_m|Y)e^{-i\alpha_m}. \quad (10.2.4)$$

In this case our wave functions in the x and z representations under knowledge Y are generally different with regard to their absolute *and* relative phases. Our phases of belief in the x_i and in the equivalent z_m are different for each value of i but our degrees of belief in the x_i and in the equivalent z_m are the same (as required by the first uniqueness principle in section 5 of Chapter I).

Results (10.2.3) and (10.2.4) are in agreement with (or served as the original reason for establishing) the general rule for phases claimed in section 5 of Chapter I.

10.3 Reasoning with certainty in combined sample spaces

Let $S^{(1)}$ and $S^{(2)}$ be closed sample spaces referring respectively to systems $S^{(1)}$ and $S^{(2)}$. If $x_i^{(1)}, y_j^{(1)}, \dots$ are a set of equivalent bases in $S^{(1)}$ and $x_n^{(2)}, y_m^{(2)}, \dots$ are a set of equivalent bases in $S^{(2)}$ then the combined bases such as $x_i^{(1)}x_n^{(2)}$ and $y_j^{(1)}y_m^{(2)}$, evidently form an equivalent set in $S^{(1)}S^{(2)}$. The transfer functions $\Phi(x_i^{(1)}x_n^{(2)}|y_j^{(1)}y_m^{(2)})$ are (for given j and m) non-zero only for one value of (i, n) . For, by the product rule for wave functions

$$\Phi(x_i^{(1)}x_n^{(2)}|y_j^{(1)}y_m^{(2)}) = \Phi(x_i^{(1)}|y_j^{(1)})\Phi(x_n^{(2)}|y_m^{(2)})$$

and the LHS is only non-zero when

$$y_j^{(1)} \Rightarrow^\alpha x_i^{(1)} \text{ and } y_m^{(2)} \Rightarrow^\beta x_n^{(2)}$$

which apply (for certain definite values of the phases α and β) only when

$$j = k_i \text{ and } m = l_n,$$

k_i and l_n being certain single valued functions of i and n . We then have

$$\Phi(x_i^{(1)}x_n^{(2)}|y_j^{(1)}y_m^{(2)}) = e^{i(\alpha+\beta)}$$

and so we find the rule

$$y_j^{(1)} y_m^{(2)} \Rightarrow^{\alpha+\beta} x_i^{(1)} x_n^{(2)} \quad \text{when} \quad y_j^{(1)} \Rightarrow^\alpha x_i^{(1)} \quad \text{and} \quad y_m^{(2)} \Rightarrow^\beta x_n^{(2)}. \quad (10.3.1)$$

This relates phases of implication in $S^{(1)}S^{(2)}$ to phases of implication in $S^{(1)}$ and $S^{(2)}$, and is in agreement with (or served originally as the reason for claiming) the addition rule for phases under conjunction (as in (2.2.1.7) of Chapter I).

10.4 Knowledge expressed as a conjunction of propositions from equivalent bases

If bases x and y are equivalent and

$$y_j^{-\alpha_j} \Leftrightarrow^{\alpha_j} x_i \quad \text{when} \quad i = k_j$$

as in (10.1.4) to (10.1.6), then x_i and y_j (with $i = k_j$) claim correlated properties of the quantum mechanical system in question and knowledge of x_i is compatible with knowledge of y_j , and therefore $x_i y_j$ (with $i = k_j$) expresses a possible state of knowledge equivalent to x_i or to y_j .

In such special cases it is possible for us to hold knowledge of the truth of propositions from different bases simultaneously. Application of the rules for phases of implication and the general rule for phases then enables us to calculate the form taken by wave functions when our pure knowledge is expressed as a conjunction of equivalent propositions taken from equivalent bases.

For example if bases y and z are equivalent as in (10.2.2) and basis x is not equivalent to y and z , then a wave function $\Phi(x_i | y_j z_m)$ (where $j = k_m$) is related to $\Phi(x_i | y_j)$ by

$$\Phi(x_i | y_j z_m) = \Phi(x_i | y_j) e^{-ik} \quad (10.4.1)$$

where k is the phase characteristic of knowledge z_m . This follows from the general result (2.2.1.20) of Chapter I which here means that $y_j^{-k} \Leftrightarrow^k y_j z_m$, giving (10.4.1) directly from the general rule for phases.

The result (10.4.1) (and many others involving conjunctions of propositions from equivalent bases) lie outside the conventional quantum mechanical formalism. They do not add any new physics but are nonetheless of interest in the present interpretation of quantum mechanics all results and deductions within which should form a consistent whole.

10.5 Consequences of the general law of reciprocity

The general law of reciprocity (section 3.11 of Chapter I) states that given propositions Y and Z claiming dynamical properties of a system S , if Y and Z could each represent (generally different) pure states of knowledge of S then the relation

$$\Phi(Y|Z) = \Phi^*(Z|Y) \quad (10.5.1)$$

must hold. Assuming Y and Z represent possible pure states of knowledge, we note the following consequences of (10.5.1) that result from the first law of extreme values of probability (section 2.2.2 of Chapter I).

(i) If acquisition of knowledge Z is known (from our general knowledge G) to bring about or ensure the truth of Y (as a result of the uncertainty principle), then $\Phi(Y|Z) = e^{i\alpha}$ where α is an indeterminate phase. And it then follows from (10.5.1) that $\Phi(Z|Y) = e^{-i\alpha}$ with indeterminate phase $-\alpha$ so we should *expect* Z to be true when we know Y is true.

(ii) If we know (from G) that $Z \Rightarrow Y$ with an indeterminate phase α , then by (10.5.1) $\Phi(Z|Y) = e^{-i\alpha}$ where the phase $-\alpha$ is indeterminate and we should again *expect* Z to be true when we know Y is true.

(iii) If we know (from G) that $Z \Rightarrow Y$ with an *determinate* phase α , then $\Phi(Y|Z) = e^{i\alpha}$ and by (10.5.1) $\Phi(Z|Y) = e^{-i\alpha}$ where the phase $-\alpha$ is determinate, so in this case $Y \Rightarrow Z$ with an determinate phase $-\alpha$. The properties claimed by Y and Z are then naturally correlated independently of any knowledge we may or may not have about the system.

CHAPTER III

LAWS OF NON-RELATIVISTIC QUANTUM MECHANICS

1. Quantum mechanical processes

Non-relativistic quantum mechanics is a theory of systems of particles in motion. Each particle maintains its form and no particles are created or destroyed. They move in ordinary (Euclidean) fixed space and ordinary (Newtonian) time.

In the present interpretation of non-relativistic quantum mechanics we adopt a picture of particles which is the same as in classical mechanics in as much as they are viewed as material points with fixed masses moving in ordinary space and time. So at each moment in time any particle has a definite position in space. It seems however that we cannot carry over the classical picture of *smooth* orbital motion of particles. So particle position coordinates are taken to be *continuous* functions of time but not *differentiable* functions of time. Particle position coordinates are therefore changing in an irregular manner at the smallest scales.

Relative to a stationary frame of reference* a system with N particles has properties with classical analogue such as particle positions (vectors $\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N$) and particle momenta (vectors $\mathbf{p}_1, \mathbf{p}_2 \dots \mathbf{p}_N$) and properties without classical analogue (like the spin s of each particle and its z component of spin in each fixed right-handed Cartesian coordinate system†). A z component of particle spin may change abruptly (discontinuously) from one allowed value to another but is almost always constant over a small enough time interval.

We assume that definite orbital and spinning motions take place determined by mechanisms unknown to us. These motions are therefore governed by laws, but these laws may not be finite in number – i.e. they may not be expressible in a finite number of propositions.

We make no claim to know the detailed laws governing the motions of systems of particles. Instead we claim to know only certain general properties of the motions and we calculate our probabilities based on this limited knowledge. We claim for example that particle motions may depend on certain unchanging properties, like particle masses and spins, and the internal system potential function, without saying how. We claim that the motion of a system over a short time interval is not at all influenced by or dependent upon the value of the system potential at *later* times. We claim (as we have said) continuity of particle orbital motion and discontinuity of particle spinning motion. Other general properties of the motions will be claimed in this Chapter and certain others will

* A frame of reference can notionally be regarded as a system of axes and synchronised clocks filling all space and made of particles of such high mass that the uncertainty principle is not of concern for them. These particles interact with each other through inter-particle potentials of their own. They behave classically and in no way interact with particles of any quantum mechanical system under study.

† Henceforth, unless otherwise stated, all Cartesian coordinate systems will be assumed to be right-handed and to employ the same units of distance and the same units of time.

be claimed at various points in the rest of the monograph where their importance will be more readily appreciated.

Because of their relatively large (ideally infinite) masses, coordinate frames can be treated classically. They can remain in known fixed positions relative to one another or can move smoothly with positions and velocities known at every instant, and they are not subject to the uncertainty principle.*

We have reason to believe (and we assume it true) that the momentum of a particle is (like its spin) an *internal* property of the particle (relative to the fixed coordinate system in question) and not a property of its drifting motion through space.† However, owing to its intimate connection with particle position (in the uncertainty principle) we *classify* it as a property of particle orbital motion. (If we try to insist on smooth differentiable particle motion and define momentum and orbital angular momentum in the classical way we will arrive at contradictions with the predictions of non-relativistic quantum mechanics.)

A system of N particles may move under the action of a (generally time-dependent) system potential $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$. This is a function of the time and of the positions $\mathbf{r}_1, \dots, \mathbf{r}_N$ of the particles relative to some stationary coordinate frame.‡ The system may move under the action of time-dependent *external* scalar and vector potential fields possibly different for each particle and specified by scalar functions $V_i(\mathbf{r}, t)$ and vector functions $\mathbf{A}_i(\mathbf{r}, t)$ $i = 1, \dots, N$ (the potential fields $V_i(\mathbf{r}, t)$ and $\mathbf{A}_i(\mathbf{r}, t)$ acting on the i^{th} particle alone). The system may move under an internal system potential and external potentials acting simultaneously.§

External fields are produced by macroscopic sources, and (like the kinematic properties of coordinate frames) the sources, and their fields are not subject to the uncertainty principle.

In addition to external fields due to sources we allow the possibility of background *constant* and *uniform* external scalar and vector fields V_0 and \mathbf{A}_0 of any magnitude and (in the case of \mathbf{A}_0) of any direction. These have no sources but act on any particle of mass m_i providing it with extra particle scalar and vector potentials of values $m_i V_0$ and $m_i \mathbf{A}_0$.** The background particle scalar potentials $m_i V_0$ and the particle scalar potentials $V_i(\mathbf{r}_i, t)$ from sources can, and often will, be included in (i.e. considered as part of) the system potential $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$, and a background particle vector potential $m_i \mathbf{A}_0$

* We should stress that it is the position and *velocity* of a coordinate system that is not subject to the uncertainty principle. The position and *momentum* of a coordinate system certainly is, but knowledge of the momentum of a coordinate system is never needed since a coordinate system serves a *kinematic* purpose only.

† See first footnote to section 2.4 of Chapter XIII.

‡ The system potential may sometimes arise from simple line-of-action particle/particle interactions and is then a function only of the distances between the particles (see section 2 of Chapter V).

§ In non-relativistic quantum mechanics there are no particle-particle interactions through inter-particle *vector* potentials.

** Being proportional to particle masses these potentials are gravitational potentials (see Appendix D) and they will play a role in the ‘quantum mechanical principle of equivalence’ (see section 3.8).

can, and often will, be included in (i.e. considered as part of) the corresponding external particle vector potential $\mathbf{A}_i(\mathbf{r}_i, t)$.

Any particle scalar potential or any system potential has units of energy and any particle vector potential has units of momentum. (The background fields \mathbf{A}_0 and V_0 above therefore have units of velocity and velocity squared respectively.) Any external vector potential field $\mathbf{A}_i(\mathbf{r}, t)$ is a divergent free (polar) vector field, so $\nabla \cdot \mathbf{A}_i(\mathbf{r}, t) = 0$.

The detailed particle motions under the action of potentials are unknown but certain general laws of potential action apply (see section 3.2). Adding a constant k to a scalar potential $V(\mathbf{r}, t)$ of a single particle or a constant vector \mathbf{K} to the vector potential $\mathbf{A}(\mathbf{r}, t)$ of that particle *does* make a difference to the quantum mechanical motion of the particle. In the classical limit the particle is expected to move according to Newton's laws in the force field $-\partial\mathbf{A}/\partial t - \nabla V + \mathbf{v} \times (\nabla \times \mathbf{A})$ where \mathbf{v} is the particle velocity.* So adding constants to $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ makes no difference to the particle motion when working only to classical accuracy.

2. Probabilistic description

2.1 Closed sample spaces and isolated quantum mechanical systems in motion

The general closed sample space \mathcal{S} is a complete sample space whose propositions refer to the detailed motion of an 'isolated' quantum mechanical system \mathcal{S} during a specified time interval t_0 to t_1 . An 'isolated' system \mathcal{S} can be a system whose motion is affected by a known external field but cannot be a system whose particles interact with particles of another system whose motions are uncertain. To be 'isolated' the system \mathcal{S} and any of its parts must also be *distinguishable* from the whole or parts of any other system. For example, if \mathcal{S} is a single particle it must be one distinguishable from any other particle either by clear spatial separation from it or on account of it being a particle of a different type from the (outside) particle which (though not part of system \mathcal{S}) might then approach close to it.†

Two quantum mechanical systems $\mathcal{S}^{(1)}$ and $\mathcal{S}^{(2)}$ each in isolated motion during a certain time interval (t_0 to t_1) can be considered together as one isolated quantum mechanical system $\mathcal{S}^{(1)}\mathcal{S}^{(2)}$ in motion during the same time interval. A closed sample space for system $\mathcal{S}^{(1)}\mathcal{S}^{(2)}$ is the combination $\mathcal{S}^{(1)}\mathcal{S}^{(2)}$ of the contemporary and closed sample spaces $\mathcal{S}^{(1)}$ and $\mathcal{S}^{(2)}$ associated with $\mathcal{S}^{(1)}$ and $\mathcal{S}^{(2)}$ respectively.

If the systems have interacted in the past (before time t_0) $\mathcal{S}^{(1)}$ and $\mathcal{S}^{(2)}$ are generally *logically dependent* - knowledge in relation to one system (or in relation to its

* The most common particle potentials are those associated with electromagnetic fields in which case $-\partial\mathbf{A}/\partial t - \nabla V + \mathbf{v} \times (\nabla \times \mathbf{A})$ is the Lorentz force. (See Appendix C.) However, we leave open the possibility also of non-electromagnetic particle potentials of both the scalar and vector variety.

† If the particles are of the same kind and come so close as to be indistinguishable on account of the 'principle of indistinguishability of identical particles' (in section 3.5), we can no longer consider either particle to constitute an 'isolated system' even if the particles are known not to interact with each other.

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sample space) is also knowledge in relation to the other. But if our knowledge in relation to $S^{(1)}$ is pure and our knowledge (simultaneously held) in relation to $S^{(2)}$ is pure then the law of absolute logical independence under pure knowledge (see section 3.7 of Chapter I) applies and $S^{(1)}$ and $S^{(2)}$ must be logically *independent*.

The possibility of combining isolated systems and the closed sample spaces associated with them extends naturally to any number of isolated systems in motion. And different aspects of one and the same quantum mechanical system (for example the orbital motion and the spinning motion of a particle) can sometimes qualify as isolated quantum mechanical systems in motion.

Finally we note the following important principle.

Principle of short-time isolation

To a limited extent a quantum mechanical system that interacts with others and/or moves in known external fields can be considered to be isolated and free from the action of the external fields. This is because actions and interactions take time to have an effect on certain properties, so *over a short enough time interval*, a moving system in interaction with another and/or under the action of external fields can be considered isolated and free of the external fields *as far as those properties are concerned*. That is, any interaction potentials and external fields can be briefly ‘switched off’ leaving those properties unaffected.*

Therefore if we reason only with propositions concerning those unaffected properties present during a short enough time period, we can proceed to apply to those propositions the laws of probability that would apply if our system was not in interaction with any others and not under the influence of external fields.†

2.2 Examples of closed sample spaces associated with isolated quantum mechanical systems in motion

Single particle in an external potential field

With regard to the orbital motion (over a specified period of time) of a single spin zero particle in a known scalar and/or vector potential field, the set of *all* propositions claiming properties of its position and momentum during the specified period form a closed sample space we denote as S_r . Each atomistic proposition of this sample space claims a specific history of the particle position and the particle momentum over the specified time period. We then have, in S_r , propositions that are disjunctions of the

* Which properties are unaffected will be part of our general knowledge G . It would seem in fact that all the most common *basic* properties like particle positions, particle momenta and the z components of particle spin, are in this category, though quantum mechanical acceleration (as defined on p.56 of [12]) evidently is not.

† In the limited context under discussion, our general knowledge regarding the interactions and external fields is then redundant.

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atomistic propositions, for example the proposition claiming just that the particle occupies a certain position at a certain time during the time period, and the proposition claiming just a certain value for the particle momentum at a certain time during the time period, and so on.

If there is no external field (so the particle moves freely) or if there is only a *uniform* external scalar and/or vector potential field, the components of motion of the particle in each of three mutually perpendicular directions x , y and z qualify as motions of ‘isolated’ quantum mechanical systems. Motion in the x direction for example is motion under the x component of the vector potential and under one-third of the 3-D uniform scalar potential. (The action of the (uniform) scalar potential is equally shared between the three component motions (as shown in section 3.1 of Chapter IV).) The set of all propositions concerning the particle position and momentum in the x direction during the specified time then form a closed sample space S_x . And similarly there are closed sample spaces S_y and S_z associated with the position and momentum in the y and z directions. These closed sample spaces can be combined to form the closed sample space $S_x S_y S_z$ associated with the motion of the particle in 3-D space, $S_x S_y S_z$ being the same as sample space S_r defined above.

If the particle has spin (and therefore an associated magnetic moment^{*}) and moves in a *uniform* (possibly time dependent) external magnetic field[†], the orbital motion has no effect on the spinning motion so the spinning motion of the particle can be considered as an ‘isolated quantum mechanical system in motion’, isolated, that is, from its orbital motion. And the set of all propositions concerning the spinning motion relative to fixed Cartesian coordinate systems in a specified time interval form a closed sample space S_σ . Similarly, since the spinning motion has no effect on the orbital motion the orbital motion can be considered as an ‘isolated quantum mechanical system in motion’, isolated, that is, from its spinning motion. And the set of all propositions concerning the orbital motion over the same time interval also form a closed sample space S_r . Thus the set of all possible propositions concerning the z components of spin *and* the orbital motion in the same time interval form a closed sample space $S_r S_\sigma$.

Two particle system

With regard to the orbital motions, in a specified time period, of two distinguishable (spin zero) particles possibly moving in their own external potentials and/or interacting through an internal system potential, the set of all propositions concerning the particle positions and momenta in the specified time period form a closed sample space $S_{r_1 r_2}$.

Formally we can write $S_{r_1 r_2} = S_{r_1} S_{r_2}$ were S_{r_1} and S_{r_2} are the separate sample spaces of propositions about the positions and momenta of particle 1 and particle 2 respectively in the same time period. If the particles are not interacting with each other

^{*} We assume a particle with non-zero spin always has a non-zero magnetic moment.

[†] i.e. in an electromagnetic vector potential whose curl is at any time uniform in space. This vector potential may affect the orbital motion if the particle is charged.

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S_{r_1} and S_{r_2} are also closed and probability rules for the combinations of closed sample spaces can be applied. As explained in section 2.1, those rules can also be applied, for a short enough time period, when the particles interact through an internal system potential because the properties of position and momentum are, for short enough times, unaffected by switching off the system potential.

2.3 Examples of bases in the above sample spaces

With regard to the sample space S_r (of section 2.2) for orbital motion of a particle under the action of a known external potential, the set of all propositions claiming that, at a certain moment in time, the particle lies in one of the infinite number of equal cubical volume elements dV filling space and represented by $dx dy dz$ in any fixed (Cartesian) coordinate system constitutes a basis. The same set of propositions referring to another time during the specified time period constitutes an alternative basis. As does the set of all propositions claiming that at that time (or at another time) the particle momentum lies in one of the infinite number of equal cubical volume elements $d^3\mathbf{p}$ ($= dp_x dp_y dp_z$) filling the momentum space associated with the coordinate system.

With regard to the sample space S_x (of section 2.2) relating to the x component of the particle motion, the set of all propositions claiming that, at one moment in time during the specified time interval, the x component of position of the particle lies in one of an infinite number of equal line elements dx filling the x axis constitutes a basis. Similarly, with reference to the same coordinates there are bases of propositions of the kind ‘ y in dy ’ or ‘ z in dz ’ at that time in the sample spaces S_y or S_z for the motions in the y or z directions respectively. These three bases may be combined to form (in sample space $S_r = S_x S_y S_z$) a basis the propositions of which claim ‘particle is in dV ’ at one moment in time (where $dV = dx dy dz$).

If the particle has spin s , then with regard to the sample space S_σ (of section 2.2) for the spinning motion of the particle, the set of all propositions claiming that at one moment in time the component σ of spin along the z axis of a fixed Cartesian coordinate system has one or other of the possible values $-s, -s+1, \dots, s-1, s$ constitutes a basis. The same set of propositions referring to another time in the specified time period or to another fixed Cartesian coordinate system constitutes an alternative basis. When the particle has an associated magnetic moment and moves in a *uniform* (possibly time dependent) external magnetic field one of the above propositional bases in S_σ can be combined with one in sample space S_r (of section 2.2) to give a basis for describing our knowledge (in the sample space $S_{\sigma r} = S_\sigma S_r$) of the process of orbital and spinning motion of the particle.

If the same particle (with its magnetic moment) moves in a *non-uniform* external magnetic field the set of propositions claiming that σ has one or other of the values $-s, -s+1, \dots, s-1, s$ at time t and the particle occupies one or other of the equal volume

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elements dV filling space at time t still constitutes a basis in sample space $S_{\sigma r}$. Here $S_{\sigma r} (= S_{\sigma} S_r)$ is closed even though S_{σ} and S_r are not.

Similarly, in sample space $S_{r_1 r_2}$ (of section 2.2) for the orbital motion of a two particle system, where the (spin zero) particles interact with each other and are not identical, the set of all propositions claiming that at one moment in time particle 1 lies in volume element dV_1 (one of an infinite number of equal cubical volume elements filling space) *and* that simultaneously particle 2 lies in a cubical volume element dV_2 constitute a basis. These propositions are fully equivalent to the propositions that claim the representative point in the (six dimensional) configuration space lies in volume element $dV_1 dV_2$ (one or other of the infinite number of equal cubical volume elements filling configuration space).

Quantum mechanical systems in motion, closed sample spaces and bases in them are many. The above examples are just a few. We know (or learn) from experience which components of a quantum mechanical system can sometimes constitute isolated moving systems, and then which sets of propositions constitute complete sample spaces (and bases in them) and how and when these sample spaces (and the bases in them) may be combined to form (closed) sample spaces containing bases suitable for describing any pure knowledge of the whole moving system.

2.4 Probability distributions and wave functions

Probability distributions that qualify as ‘wave functions’ (see section 3.3 of Chapter I) are the same (except for an infinitesimal factor in the case of bases with continuous parameters) as the wave functions in the usual quantum mechanical formalism.

For example, for a single (spin zero) particle at one moment in time, a pure state probability distribution $\Phi(dV|Y)$ over position in a fixed coordinate system is related to the usual wave function $\psi(\mathbf{r})$, by

$$\Phi(dV|Y) = \psi(\mathbf{r}) \sqrt{dV} \quad (2.4.1)$$

where, on the left, dV = ‘particle is in volume element dV ’ and Y is our pure (or essentially pure) knowledge concerning the particle motion. And on the right \mathbf{r} denotes the particle position (or rather the position of dV).^{*} The square root on the right is clearly needed in connection with the required normalisation:

$$\sum_{dV} |\Phi(dV|Y)|^2 = \int |\psi(\mathbf{r})|^2 dV = 1 \quad (2.4.2)$$

^{*} When our knowledge Y is not necessarily pure $\Phi(dV|Y)$ still takes the form (2.4.1) and (2.4.2) still applies but the phase or argument $\angle \psi(\mathbf{r})$ of $\psi(\mathbf{r})$ may no longer be determinate.

Note that we will continue to use the term ‘wave function’ for functions (like $\psi(\mathbf{r})$ in (2.4.1)) that are called wave functions in the usual formulation of quantum mechanics, or sometimes, when appropriate, we will call them ‘probability densities’ not forgetting they must be multiplied by the *square-root* of the volume element of configuration space to turn them into (complex-valued) probabilities.

3. Physical laws of quantum mechanics

3.1 Law of continuous motion

Particles move continuously in space always taking some time to traverse a distance. They cannot pass from one point to another infinitely fast. So the distance moved by a particle in a non-zero but short enough time τ is for certain less than any pre-assigned distance Δ .

3.2 Laws of potential action

With regard to the orbital motion of particles we claim the following laws of potential action.

In relation to particle positions in fixed space as functions of time, we claim the ‘first law of potential action’:

First law

The orbital motion of a particle under the action of an external scalar potential (specified by a function $V(\mathbf{r}, t)$ of time t and position \mathbf{r} in a fixed coordinate system) is different from its motion under no such potential. In any short time interval t to $t+dt$ its motion is dependent upon the local potential (i.e. on the value of $V(\mathbf{r}, t)$ at the position occupied by the particle, zero potential having no effect on the motion) but it is not dependent on the values of $V(\mathbf{r}, t)$ at other places or on the local gradient (first spatial derivatives) of the potential or on the time derivative of the potential (or on higher spatial and time derivatives of the potential) during the time interval.* Nor is it dependent on values of $V(\mathbf{r}, t)$ anywhere at times *after* time $t+dt$. It may however be dependent on values of $V(\mathbf{r}, t)$ at positions \mathbf{r} that (given our knowledge of its motion) the particle might have occupied before time t .†

* That is, the effects of the momentary local higher (spatial or temporal) derivatives of $V(\mathbf{r}, t)$ are of order dt^2 or higher, while the order of the effect of the momentary local value of $V(\mathbf{r}, t)$ is of order dt .

† This latter dependence seems evident, for example, in an interferometer for an electron (where the mirrors (‘half-silvered’ or ‘ordinary’) are potential barriers). If the ordinary mirror in one path (say mirror M in Figure 1.3.1 of Chapter XII) is removed, the electron may pass (via the other path) through the final (half-silvered) mirror in a direction it never takes when mirror M is present. We seem here to have delayed

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This law generalises to a *system* of particles under the action of any system potential specified by a function $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ of time t and the positions $\mathbf{r}_1, \dots, \mathbf{r}_N$ of all the particles in a fixed coordinate system (i.e. the position of the representation point in configuration space). The orbital motions are, in any short time t to $t + dt$, affected by the value of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ at the position occupied by the representation point, but not by the value of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ at other positions or by the local gradient (first spatial derivatives) of the potential in configuration space* or by the time derivative of the potential (or by higher spatial and time derivatives of the potential) and not by $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ after time $t + dt$. It may however be affected by the values of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ at points of configuration space that might have been occupied before time t .

First law (cont.)

The orbital motion of a particle under the action of an external *vector* potential specified by a function $\mathbf{A}(\mathbf{r}, t)$ of time t and position \mathbf{r} relative to fixed coordinates is, in any short time t to $t + dt$, affected by a non-zero value of $\mathbf{A}(\mathbf{r}, t)$ at the position occupied by the particle but not by $\mathbf{A}(\mathbf{r}, t)$ at other places and not by the local gradient (first spatial derivatives) of $\mathbf{A}(\mathbf{r}, t)$ or by the time derivative of $\mathbf{A}(\mathbf{r}, t)$ (or by higher spatial and time derivatives of $\mathbf{A}(\mathbf{r}, t)$) nor by the form of $\mathbf{A}(\mathbf{r}, t)$ after time $t + dt$. It may however be affected by $\mathbf{A}(\mathbf{r}, t)$ at places where the particle might have been before time t .

With regard to effects of the motion of sources on the fields they generate we claim ‘the second law of potential action’:

Second law

Let $V_i(\mathbf{r}, t)$ and $\mathbf{A}_i(\mathbf{r}, t)$ be the external scalar and vector potential fields of (macroscopic) sources acting on the i^{th} particle of a quantum mechanical system.

If the source of $V_i(\mathbf{r}, t)$ is moved at constant velocity \mathbf{v} relative to fixed space but still occupies the same position as before at time $t = 0$, and if the source is unaffected internally, then its field moves along with it, i.e. $V_i(\mathbf{r}, t)$ changes to $V_i(\mathbf{r} - \mathbf{v}t, t)$.

action by the potential of mirror M (at the time the electron might have struck it) on the motion of the electron through the final half-silvered mirror. (For an alternative view see section 4 of Chapter XV.)

* This situation is quite different from the situation in classical mechanics, where it is of course precisely the first spatial derivatives of the potential (the forces) that affect the motion. In quantum mechanics potential is therefore more fundamental than force. Adding a constant to the potential in quantum mechanics can make a difference to the particle motions whereas adding a constant to the potential in classical mechanics makes no difference at all to particle motions.

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If the source of $A_i(\mathbf{r}, t)$ is moved at constant velocity \mathbf{v} relative to fixed space, occupies the same position as before at time $t = 0$, and is unaffected internally, then its field too moves along with the source, so that $A_i(\mathbf{r}, t)$ changes to $A_i(\mathbf{r} - \mathbf{v}t, t)$, but the source also gives rise to an additional *scalar* potential field $\Delta V_i(\mathbf{r}, t)$ of value $\mathbf{v} \cdot \mathbf{A}_i(\mathbf{r} - \mathbf{v}t, t)$ acting on the i^{th} particle.*

Finally, with regard to the rate of increase of the *momenta* of particles relative to a fixed coordinate system we claim ‘the third law of potential action’:

Third Law

Relative to a fixed coordinate system, the momentum of a particle in an external scalar potential (specified by a function $V(\mathbf{r}, t)$ of time t and position \mathbf{r} in our coordinate system) changes as follows. In any short time interval t to $t + dt$ the momentum is increased at a rate proportional to the momentary local gradient $\nabla V(\mathbf{r}, t)$ of the potential at the position occupied by the particle, a spatially uniform potential having no effect on the momentum. But the momentum is not dependent on the value of $V(\mathbf{r}, t)$ or on its gradient at other places or on higher spatial derivatives of $V(\mathbf{r}, t)$ at the position occupied by the particle or on the time derivatives $V(\mathbf{r}, t)$ of any order. Nor is it dependent on values of $V(\mathbf{r}, t)$ anywhere at times *after* time $t + dt$. It may however be dependent on values of $\nabla V(\mathbf{r}, t)$ at positions \mathbf{r} that (given our knowledge of its motion) the particle might have occupied before time t .

This law, like the first, generalises to a system of particles under the action of any system potential specified by a function $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ of time t and positions $\mathbf{r}_1, \dots, \mathbf{r}_N$ of all the particles in a fixed coordinate system (i.e. the position of the representation point in configuration space). Each particle momentum (relative to the coordinate system) is in any short time t to $t + dt$ increased at a rate proportional to the local gradient of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ with respect to the corresponding particle (vector) coordinate, but the particle momenta are not affected by the value of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ itself or by spatial derivatives of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ higher than the first and not by $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ after time t . They may be affected by the respective gradients of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ at points of configuration space that might have been occupied before time t .

* If a second boost \mathbf{v}' is given to the source of the vector potential, this scalar potential (like external scalar potentials in general) changes to $\mathbf{v} \cdot \mathbf{A}_i(\mathbf{r} - \mathbf{v}t - \mathbf{v}'t, t)$ and a new scalar potential $\mathbf{v}' \cdot \mathbf{A}_i(\mathbf{r} - \mathbf{v}t - \mathbf{v}'t, t)$ is added. The result is the same as that of a single boost $\mathbf{v} + \mathbf{v}'$. Note that the second law of potential action can, in the case of electromagnetic potentials, be derived from electromagnetic field theory (see Appendix C).

Third law (cont.)

Relative to a fixed coordinate system, the momentum of a particle under the action of an external vector potential specified by a function $A(\mathbf{r},t)$ of time t and position \mathbf{r} relative to the fixed coordinates is, in any short time t to $t+dt$, increased at a rate proportional to the momentary first spatial derivatives of $A(\mathbf{r},t)$ at the position occupied by the particle at time t . Its rate of increase is not affected by the local value of $A(\mathbf{r},t)$ itself or by the local spatial derivatives of $A(\mathbf{r},t)$ higher than the first, or by the time derivatives of $A(\mathbf{r},t)$ (of any order) nor by the form of $A(\mathbf{r},t)$ after time $t+dt$. It may however be affected by the spatial gradients of $A(\mathbf{r},t)$ at places where the particle might have been before time t .

3.3 Fundamental unit of action

In non-relativistic quantum mechanics there is just one fundamental unit - the unit of action \hbar ($=1.05459\times 10^{-34}$ Js).

3.4 Correspondence principle

Under ‘quasi-classical’ states of pure knowledge of a process in quantum mechanics, particles are expected to move (to classical accuracy) in classical orbits. And the moduli squared of the probabilities of propositions concerning properties with a classical analogue (calculated using the rules of complex-valued probability and the physical laws of quantum mechanics and averaged if necessary over classically small domains) must be interpretable as classical probability distributions over classical properties consistent with the laws of classical mechanics and classical probability.

3.5 Principle of indistinguishability of identical particles

Except in special cases, it is impossible for us to mark, keep track of, or recover the identity of two or more identical particles (e.g. two or more electrons) that interact with one another at the quantum level.

Of course when we say ‘impossible for us’ we mean it is impossible using macroscopic instruments (natural or manmade) to project a macroscopic image that would enable us to keep track of identical particles or recover their identity during or after their interaction at the quantum level. In special cases some distinctive features of the particles (e.g. their (different) spin components in a certain direction) may be known to us and may be

known to remain constant during interaction, then measurement of these at any time during or after the interaction *could* enable us to learn which particle was which.

3.6 Assumption of natural ordering of particles and systems of particles

It is supposed that nature herself, so to speak, *can and does* keep track of all particles (including identical particles) even if they interact at the quantum level without maintaining what we could recognise as distinctive features. So she always ‘knows’ which is which.

We also suppose that particles and systems of particles are (once and for all time) ordered or numbered by nature in a random way (i.e. in a way completely unknown to us).*

We do not know the ordering scheme and there is no way we can learn it, but in connection with non-identical particles or systems, claiming one particular ordering scheme (rather than another) never leads to disagreement between theoretical predictions and experimental results.

In the case of identical particles or identical systems it is possible to claim to know the natural order of *them* only in connection with processes during which the particles or systems *remain clearly distinguishable throughout* (on account of their spatial separation for example). In that limited context claiming one particular ordering scheme (rather than another) never leads to disagreement between theoretical predictions and experimental results.

3.7 Bosons and fermions and the inter-penetrability of all particles

Particles are divided into two classes called ‘bosons’ and ‘fermions’ according as their spins are integral (have one of the values 0,1,2,...) or half-integral (have one of the values $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$).

Any number of particles (whether or not some are identical) may occupy the same infinitesimal volume element of space regardless of their z components of spin. So the probability of this happening is never zero for *physical* reasons. It *is* zero in the case of identical fermions whose z components of spin (relative to a fixed coordinate system) are known to be equal, but this comes about for logical reasons rather than physical reasons as will be explained in Chapter X.

* This natural numbering (or ordering) is needed to allow the possibility of a natural ordering of the propositions of bases concerning spin components of more than one particle and to demonstrate the symmetry properties of wave functions for systems of particles some of which are identical.

3.8 Lack of knowledge with regard to fixed space and background fields, and the quantum mechanical principle of equivalence

As in classical mechanics, we claim that there is no way we can know whether or not a particular inertial frame is at rest with respect to fixed space.* No experiment can settle such a question. We are also ignorant with regard to the values of the background fields V_0 and \mathbf{A}_0 that may be present in fixed space and we claim that no experiment can reveal their values.

Therefore, without contradiction with experiments, we may *assume* that any particular inertial frame O is at rest and take any particular values V_0 and \mathbf{A}_0 for the background fields.† But for future use we lay down the following principle.

Quantum mechanical principle of equivalence

Although we do not know the detailed laws that govern the orbital and spinning motions of particles, we claim that under those laws *exactly the same motions* (relative to any coordinate system) could occur if instead of frame O the property of being at rest was held by a frame O' moving at a constant velocity \mathbf{v} with respect to O and additional background fields ΔV_0 and $\Delta \mathbf{A}_0$ were present with values $\Delta V_0 = -\frac{1}{2}\mathbf{v}^2 - \mathbf{v} \cdot \mathbf{A}_0$ and $\Delta \mathbf{A}_0 = \mathbf{v}$ respectively causing an additional scalar potential $\Delta V_i = -\frac{1}{2}m_i\mathbf{v}^2 - \mathbf{v} \cdot (m_i\mathbf{A}_0)$ to act on each particle (m_i being the mass of the particle) and an additional vector potential $\Delta \mathbf{A}_i = m_i\mathbf{v}$ to act on each particle (m_i being again the mass of the particle).‡

3.9 The ‘spinorial’ character of coordinate systems

The group of rotations of a coordinate system, or of any (classical) rigid body, is assumed to be the group $SU(2)$ (rather than the group $SO(3)$). Thus a coordinate system (or any rigid body) has two ways of occupying any specific orientation in space. We can get from one to the other by making one full turn of the coordinate system (or the rigid body) in either direction about any axis. Two full turns of a coordinate system (or of any rigid body) about an axis always returns it to the same state.

* Since coordinate frames and particles of large enough mass behave classically, an inertial frame in quantum mechanics can be defined, as in classical mechanics, as a system with respect to which any free particle of large enough mass remains at rest or moves uniformly in a straight line.

† Lack of knowledge with regard to fixed space and the background fields is not a consequence of the uncertainty principle; therefore we are at liberty to suppose we know which inertial frame is representative of fixed space and what background fields are present without violating the uncertainty principle.

‡ The quantum mechanical principle of equivalence resembles the principle of equivalence in classical mechanics (employed in general relativity). The latter principle asserts that a uniformly *accelerating* coordinate system can be considered to be at rest provided a certain extra uniform gravitational field is supposed to occupy all space. Here too exactly the same particle motions (relative to any coordinate system) take place (under the same initial conditions).

III. *Laws of non-relativistic quantum mechanics*

We suppose there is meaning to the question as to whether or not two coordinate systems (or similar rigid bodies) in the same orientation occupy that orientation in the same way. If they do not, a full rotation of either ensures they do. Coordinate systems (or similar rigid bodies) that move and turn around so they may have any positions in space but always the same orientation as each other maintain the sameness or difference in the way they occupy their orientations.

Suppose two coordinate systems (or similar rigid bodies) have initially the same orientation as each other. They may occupy that orientation in the same way or in a different way – they may be in a state of sameness or difference in that regard. Suppose they then move and turn around in any manner (independently of each other) but finally have again the same orientation as each other (possibly an orientation different from the initial one). Then it is possible to apply a test (we will call it the ‘band test’) to see whether or not they come to occupy their final orientation in the same state of sameness or difference as applied initially. In the band test the two coordinate systems (or similar rigid bodies) are initially joined by a flexible band (for example an elastic neck tie) one end of which is rigidly attached to one body and the other end of which is rigidly attached to the other body. If, and only if, the state of twist of the band (modulo slipping the band over either body any number of times) is ultimately the same, the bodies have returned to the same state of sameness or difference with regard to the way they occupy their common orientation (see p. 205 of [11]).

3.10 Absence of observable consequences of a full rotation of coordinates

We cannot know, on any particular occasion, whether coordinate systems of the same orientation occupy that orientation in the same way or not, but we are at liberty to assume they do or do not as we please. Then if the coordinate systems are moved and turned around we should of course use the band test (or its equivalent) to determine if they are occupying the same orientation in the same way on a different occasion. But even if we neglect to apply the band test and become unsure at a later time whether two parallel coordinate systems are occupying their common orientation in the same way or not and have to guess, it will not matter. That is, there are no observable consequences that would reveal a wrong choice.*

3.11 The isotropy of space, the homogeneity of space and time, time reversal and inversion

Consider the quantum mechanical motion of a system of particles moving under the action of an internal system potential, external potentials due to macroscopic sources, a background scalar field V_0 and a background vector field A_0 . We do not know the detailed laws governing the motion of the particles, but in the absence of a background

* Lack of knowledge of the way coordinate systems occupy their orientations is not a consequence of the uncertainty principle. We are thus at liberty to suppose we know whether parallel coordinate systems occupy their common orientation in the same way or not without violating the uncertainty principle.

III. Laws of non-relativistic quantum mechanics

vector field, i.e. with $A_0 = 0$, or equivalently with additional (unchanging) vector potentials applied by us to cancel out the action of A_0 on each particle, we suppose the following laws hold good.

Law of isotropy of space and homogeneity of space and time

For every possible macroscopic source history and every possible motion of a particle system (in the fields of the sources) relative to a certain fixed Cartesian coordinate system, an identical source history and system motion relative to any other fixed Cartesian coordinate system is a possibility. (Here we allow the zero point in time also to be different in the two coordinate systems.)*

The motion of the particle system may include spinning motion of the particles as well as orbital motion of them. Then both the orbital and spinning motions of the particles are the same relative to the respective coordinate systems. So the x, y and z components of position of each particle are the same functions of time, and the z components of spin of each particle are the same functions of time in the respective coordinate systems. Because of this, we have no reason to attach special significance to any particular (fixed) coordinate system and this is what we mean when we say that space is homogeneous and isotropic and time is homogeneous.†

Law of time reversal

Relative to fixed space, for every possible macroscopic source history and every possible motion of a particle system in the fields of the sources a time reversed source history and particle motion is a possibility.

Under time reversal some of the dynamical variables with a classical analogue change sign while others stay the same. Thus, taking time reversal through the time origin ($t = 0$), the positions and momenta of the i^{th} particle and the internal system potential function change as follows

$$\begin{aligned} \mathbf{r}_i(t) &\rightarrow \mathbf{r}_i(-t), \\ \mathbf{p}_i(t) &\rightarrow -\mathbf{p}_i(-t), \\ V(\mathbf{r}_1, \dots, \mathbf{r}_N, t) &\rightarrow V(\mathbf{r}_1, \dots, \mathbf{r}_N, -t). \end{aligned} \tag{3.11.1}$$

* Put another way, every particle system together with the macroscopic sources serving it may be advanced or retarded in time and bodily translated and rotated to a new location in fixed space and still function in exactly the same manner.

† Of course if a non-zero background vector field A_0 is present and is not cancelled out, space and time are still homogeneous but space is no longer isotropic, or only isotropic with regard to rotations about the direction of A_0 .

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The ‘time reversed source history’ is one in which the original external scalar and vector potential fields $V_i(\mathbf{r}, t)$ and $\mathbf{A}_i(\mathbf{r}, t)$ for each particle and the magnetic field $\mathbf{H}(\mathbf{r}, t)$ have changed as follows.*

$$\begin{aligned} V_i(\mathbf{r}, t) &\rightarrow V_i(\mathbf{r}, -t), \\ \mathbf{A}_i(\mathbf{r}, t) &\rightarrow -\mathbf{A}_i(\mathbf{r}, -t), \\ \mathbf{H}(\mathbf{r}, t) &\rightarrow -\mathbf{H}(\mathbf{r}, -t) \end{aligned} \tag{3.11.2}$$

Under time reversal the z components of spin in any fixed Cartesian coordinate frame O simply change sign. Thus for all i and in any one coordinate frame O

$$\sigma_i(t) \rightarrow -\sigma_i(-t). \tag{3.11.3}$$

But it is important to state or claim, as we do, that the spinning motions relative to any fixed coordinate frame O are, under time reversal, exactly the same as the spinning motions relative to the coordinate frame \tilde{O} formed by rotating the coordinate frame O through angle π about its y axis. This is of course consistent with all the z components of spin changing sign, as in (3.11.3), but it says more because it refers to *all* aspects of the spinning motion, which are not (we suppose) captured completely by the values of the σ_i in all fixed coordinate frames.

Any process time reversed twice is the same as the original process.

Law of inversion

Relative to fixed space, for every possible source history and particle motion an inverted source history and particle motion is a possibility.

Under inversion some of the dynamical variables with a classical analogue change sign while others stay the same. Thus, taking inversion through the origin of a fixed coordinate frame, the positions and momenta of the i^{th} particle change as follows and the internal system potential changes accordingly:

* If (constant) parts of the $\mathbf{A}_i(\mathbf{r}, t)$ are used to cancel out the effects of a background vector potential \mathbf{A}_0 we should not of course change the sign of those parts. So the second of (3.11.2) refers to the external vector potentials without those parts. In the case of external *electromagnetic* potentials the time reversed forms of V_i and \mathbf{A}_i in (3.11.2) follow from the field equations governing the potentials (Appendix C) when the source motions and current directions are reversed. And the third of (3.11.2) clearly follows from the second since \mathbf{H} is the curl of the electromagnetic vector potential. In the case of non-electromagnetic potentials the time reversed forms of V_i and \mathbf{A}_i in (3.11.2) must follow when the source motions are reversed and certain other internal changes are made to the sources analogous to the reversal of the currents in the electromagnetic case.

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$$\begin{aligned}
 \mathbf{r}_i(t) &\rightarrow -\mathbf{r}_i(t), \\
 \mathbf{p}_i(t) &\rightarrow -\mathbf{p}_i(t), \\
 V(\mathbf{r}_1, \dots, \mathbf{r}_N, t) &\rightarrow V(-\mathbf{r}_1, \dots, -\mathbf{r}_N, t).
 \end{aligned}
 \tag{3.11.4}$$

The ‘inverted source history’ is one in which the original external scalar and vector potential fields $V_i(\mathbf{r}, t)$ and $\mathbf{A}_i(\mathbf{r}, t)$ for each particle, and the magnetic field $\mathbf{H}(\mathbf{r}, t)$, have changed as follows.*

$$\begin{aligned}
 V_i(\mathbf{r}, t) &\rightarrow V_i(-\mathbf{r}, t), \\
 \mathbf{A}_i(\mathbf{r}, t) &\rightarrow -\mathbf{A}_i(-\mathbf{r}, t), \\
 \mathbf{H}(\mathbf{r}, t) &\rightarrow \mathbf{H}(-\mathbf{r}, t)
 \end{aligned}
 \tag{3.11.5}$$

The z components of spin remain the same on inversion, i.e. for all i and for all fixed coordinate frames

$$\sigma_i(t) \rightarrow \sigma_i(t)
 \tag{3.11.6}$$

and all aspects of the spinning motion stay the same as well.

Any process inverted twice is the same as the original process.

* Again, we should not of course change the (constant) parts of the $\mathbf{A}_i(\mathbf{r}, t)$ used to cancel out the action of a background vector field \mathbf{A}_0 . So the second of (3.11.5) refers to the external vector potentials without those parts. In the case of external *electromagnetic* potentials the inverted forms of V_i and \mathbf{A}_i follow from the field equations governing the potentials (Appendix C) when the source motions and currents are inverted.

CHAPTER IV

DERIVATION OF THE SCHRÖDINGER EQUATION FOR THE ORBITAL MOTION OF A PARTICLE

Throughout Chapter IV arguments are conducted in the closed sample space S_r (of section 2.2 of Chapter III) referring to the position and momentum of the particle in a certain time period, or sometimes in the component sample spaces S_x, S_y and S_z (of section 2.2 of Chapter III) when they are closed. The *bases* used are the sets of propositions claiming one or other particle position at one time or another.

1. Derivation of the position/position transformation functions for a free particle

We consider all space to be divided into equal cubical elements $d^3\mathbf{r}$ labelled by their positions \mathbf{r} in a rest frame and we seek the transformation functions $\Phi(d^3\mathbf{r}_2t_2|d^3\mathbf{r}_1t_1)$ and $\Phi(d^3\mathbf{r}_1t_1|d^3\mathbf{r}_2t_2)$. The first of the transformation functions is the probability that at a time t_2 the particle lies in coordinate volume element $d^3\mathbf{r}_2$ at position \mathbf{r}_2 given the particle is known to lie in coordinate volume element $d^3\mathbf{r}_1$ at position \mathbf{r}_1 at time t_1 . The second is the probability that at a time t_1 the particle lies in coordinate volume element $d^3\mathbf{r}_1$ at position \mathbf{r}_1 given the particle is known to lie in coordinate volume element $d^3\mathbf{r}_2$ at position \mathbf{r}_2 at time t_2 .^{*} The transformation functions have the form

$$\Phi(d^3\mathbf{r}_2t_2|d^3\mathbf{r}_1t_1) = \tilde{\Phi}_{r_1t_1}(\mathbf{r}_2t_2)\sqrt{d^3\mathbf{r}_2}, \quad \Phi(d^3\mathbf{r}_1t_1|d^3\mathbf{r}_2t_2) = \tilde{\Phi}_{r_2t_2}(\mathbf{r}_1t_1)\sqrt{d^3\mathbf{r}_1}. \quad (1.1)$$

where $\tilde{\Phi}_{r_1t_1}(\mathbf{r}_2t_2)$ is a continuous differentiable function of $\mathbf{r}_1, \mathbf{r}_2, t_1$, and t_2 independent of $d^3\mathbf{r}_2$ and $\tilde{\Phi}_{r_2t_2}(\mathbf{r}_1t_1)$ is a continuous differentiable function of $\mathbf{r}_1, \mathbf{r}_2, t_1$, and t_2 independent of $d^3\mathbf{r}_1$.

The reciprocity of transformation functions gives

$$\tilde{\Phi}_{r_2t_2}(\mathbf{r}_1t_1)\sqrt{d^3\mathbf{r}_1} = \left(\tilde{\Phi}_{r_1t_1}(\mathbf{r}_2t_2)\sqrt{d^3\mathbf{r}_2}\right)^*$$

^{*} The times t_1 and t_2 must of course lie in the time period covered by the sample space S_r .

or

$$\frac{\tilde{\Phi}_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)}{\sqrt{d^3 \mathbf{r}_2}} = \left(\frac{\tilde{\Phi}_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)}{\sqrt{d^3 \mathbf{r}_1}} \right)^*.$$

Denoting the LHS by $\Phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)$ and the RHS (before conjugation) by $\Phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$ we have

$$\tilde{\Phi}_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2) = \Phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2) \sqrt{d^3 \mathbf{r}_1}, \quad \tilde{\Phi}_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1) = \Phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1) \sqrt{d^3 \mathbf{r}_2}. \quad (1.2)$$

where $\Phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$ and $\Phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)$ are continuous differentiable functions of \mathbf{r}_1 , \mathbf{r}_2 , t_1 and t_2 , and are independent of $d^3 \mathbf{r}_2$ and $d^3 \mathbf{r}_1$. So by (1.1) and (1.2)

$$\begin{cases} \Phi(d^3 \mathbf{r}_2 t_2 | d^3 \mathbf{r}_1 t_1) = \Phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2) \sqrt{d^3 \mathbf{r}_1} \sqrt{d^3 \mathbf{r}_2}, \\ \Phi(d^3 \mathbf{r}_1 t_1 | d^3 \mathbf{r}_2 t_2) = \Phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1) \sqrt{d^3 \mathbf{r}_2} \sqrt{d^3 \mathbf{r}_1} \end{cases} \quad (1.3)$$

with

$$\Phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1) = \Phi_{\mathbf{r}_1 t_1}^*(\mathbf{r}_2 t_2) \quad (1.4)$$

We will call $\Phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$ and $\Phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)$ ‘transformation functions’ even though they are only related to the actual transformation functions through equation (1.3). Note that it does not matter whether t_1 is earlier or later than t_2 . For the sake of being definite however we suppose for the time being that $t_1 < t_2$.

We are assuming that the particle moves freely i.e. in the absence of any potentials during the time period of the sample space and we find the forms of $\Phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$ and $\Phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)$ using the method of transformation groups and noting the requirements of dimensionality. But first we bring in the initial condition

$$\begin{aligned} \Phi(d^3 \mathbf{r}_2 t_2 | d^3 \mathbf{r}_1 t_1) \Big|_{t_2 \rightarrow t_1} &= \Phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2) \Big|_{t_2 \rightarrow t_1} \sqrt{d^3 \mathbf{r}_1} \sqrt{d^3 \mathbf{r}_2} \\ &= \begin{cases} 1 & \mathbf{r}_2 \text{ inside } d^3 \mathbf{r}_1 \text{ (i.e. } d^3 \mathbf{r}_2 \text{ the same as } d^3 \mathbf{r}_1) \\ 0 & \mathbf{r}_2 \text{ outside } d^3 \mathbf{r}_1 \text{ (i.e. } d^3 \mathbf{r}_2 \text{ different from } d^3 \mathbf{r}_1) \end{cases} \end{aligned}$$

which must hold because the propositional implication $d^3 \mathbf{r}_1 t_1 \Rightarrow^0 d^3 \mathbf{r}_1 t_2$ applies in the limit $t_2 \rightarrow t_1$ on account of the law of continuous motion (see section 3.1 of Chapter III). This means

IV. Derivation of the Schrödinger equation

$$\phi_{r_1 t_1}(\mathbf{r}_2 t_2) \Big|_{t_2 \rightarrow t_1} = \delta(\mathbf{r}_2 - \mathbf{r}_1) = \delta(\mathbf{R}) = \delta(x)\delta(y)\delta(z) \quad (1.5)$$

where $\mathbf{R} = \mathbf{r}_2 - \mathbf{r}_1$, where x , y and z are the Cartesian components of \mathbf{R} , and where the delta function $\delta(\mathbf{r}_2 - \mathbf{r}_1)$ is the weighted Kronecker delta function $(d^3 \mathbf{r}_1)^{-1} \delta_{d^3 \mathbf{r}_1, d^3 \mathbf{r}_2}$ i.e. a function which is zero when \mathbf{r}_2 lies outside $d^3 \mathbf{r}_1$, and equal to $1/d^3 \mathbf{r}_1$ when \mathbf{r}_2 lies inside $d^3 \mathbf{r}_1$.*

Now we note that the transformation functions $\phi_{r_1 t_1}(\mathbf{r}_2 t_2)$ and $\phi_{r_2 t_2}(\mathbf{r}_1 t_1)$ must be independent of the position of the origin of the fixed coordinate system and of the origin of the time coordinate. For under any displacement of the origin of the space coordinates and any displacement of the time coordinate origin, the distributions $\phi'_{r_1 t_1}(\mathbf{r}_2 t_2)$ in the new coordinate system must, by the homogeneity of space and time and the similarity principle (section 5.1 of Chapter I), be the same functions as the $\phi_{r_1 t_1}(\mathbf{r}_2 t_2)$ in the original coordinates except perhaps for a constant phase factor $e^{i\alpha}$ independent of $\mathbf{r}_1 t_1$ and $\mathbf{r}_2 t_2$.[†] But when $t_2 \rightarrow t_1$ both $\phi'_{r_1 t_1}(\mathbf{r}_2 t_2)$ and $\phi_{r_1 t_1}(\mathbf{r}_2 t_2)$ must be the same (both equal to $\delta(\mathbf{r}_2 - \mathbf{r}_1)$ as in the RHS of (1.5)) and therefore α can only be zero.

Use of the transformation group of displacements of the coordinate system (or of the system itself) in time and space:

Starting with a fixed coordinate system O let us make a displacement \mathbf{A} of the origin of the coordinates and a displacement δ of the time origin to give a new coordinate system O' . Then a time labelled t in O becomes a time $t' = t - \delta$ in O' and a position labelled \mathbf{r} in O becomes $\mathbf{r}' = \mathbf{r} - \mathbf{A}$ in O' . We have seen that our transformation functions in the original and in the new coordinates must be the same, i.e.

* With this definition of the delta function $\delta(\mathbf{r}_2 - \mathbf{r}_1)$ we have both normalisation of $\delta(\mathbf{r}_2 - \mathbf{r}_1)$, i.e.

$$\int \delta(\mathbf{r}_2 - \mathbf{r}_1) d^3 \mathbf{r}_2 = \sum_{d^3 \mathbf{r}_1} (d^3 \mathbf{r}_1)^{-1} \delta_{d^3 \mathbf{r}_1, d^3 \mathbf{r}_2} d^3 \mathbf{r}_2 = 1 \text{ and normalisation of the wave function}$$

$$\phi_{r_1 t_1}(\mathbf{r}_2 t_2) \Big|_{t_2 \rightarrow t_1} \sqrt{d^3 \mathbf{r}_1}, \text{ i.e. } \int \left| \phi_{r_1 t_1}(\mathbf{r}_2 t_2) \Big|_{t_2 \rightarrow t_1} \sqrt{d^3 \mathbf{r}_1} \right|^2 d^3 \mathbf{r}_2 = \sum_{d^3 \mathbf{r}_1} \left| (d^3 \mathbf{r}_1)^{-1} \delta_{d^3 \mathbf{r}_1, d^3 \mathbf{r}_2} \right|^2 d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 = 1.$$

[†] Note that the homogeneity of time is not jeopardised by the existence of the fixed times (say t_0 and t_3) marking the beginning and end of the period covered by the sample space S_r . We could if we liked let $t_0 \rightarrow -\infty$ and $t_3 \rightarrow \infty$. But the times t_0 and t_3 are anyway not relevant to the calculation of the position/position transformation functions because, as noted in section 3.2 of Chapter I, knowledge of any potentials present before time t_0 is redundant, and potentials after time t_3 have no effect. Hence *similarity* applies and gives $\phi'_{r_1 t_1}(\mathbf{r}_2 t_2) = \phi_{r_1 t_1}(\mathbf{r}_2 t_2) e^{i\alpha}$ which follows from (5.1.2) of Chapter I in the case of common general knowledge (i.e. with $G_j^{(1)} = G_j^{(2)} = G_j$) j labelling the propositions $\mathbf{r}_1 t_1$ (or $d^3 \mathbf{r}_1 t_1$) and i the propositions $\mathbf{r}_2 t_2$ (or $d^3 \mathbf{r}_2 t_2$).

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$$\phi'_{r'_1}(\mathbf{r}_2 t_2) = \phi_{r_1}(\mathbf{r}_2 t_2).$$

And since propositions claiming the same event* using different coordinate systems are fully equivalent, we have, by the second uniqueness principle (section 5 of Chapter I) that

$$\phi'_{r'_1}(\mathbf{r}'_2 t'_2) = \phi_{r_1}(\mathbf{r}_2 t_2)$$

where $t'_1 = t_1 - \delta$, $t'_2 = t_2 - \delta$, $\mathbf{r}'_1 = \mathbf{r}_1 - \mathbf{A}$ and $\mathbf{r}'_2 = \mathbf{r}_2 - \mathbf{A}$. Combining these relations we get

$$\phi_{r_1 - \mathbf{A}, t_1 - \delta}(\mathbf{r}_2 - \mathbf{A}, t_2 - \delta) = \phi_{r_1}(\mathbf{r}_2 t_2)$$

which, being true for all δ and \mathbf{A} , implies

$$\phi_{r_1}(\mathbf{r}_2 t_2) = F(\mathbf{R}, \tau). \quad (1.6)$$

where

$$\mathbf{R} = \mathbf{r}_2 - \mathbf{r}_1, \quad \tau = t_2 - t_1. \quad (1.7)$$

The same result (1.6) follows using the transformation group of displacements δ and Δ of the *system* in time and space. Here the problems of finding the probability distributions $\phi_{r_1}(\mathbf{r}_2 t_2)$ and $\phi_{r'_1}(\mathbf{r}'_2 t'_2)$ (where $\mathbf{r}'_1 = \mathbf{r}_1 + \Delta$, $\mathbf{r}'_2 = \mathbf{r}_2 + \Delta$, $t'_1 = t_1 + \delta$ and $t'_2 = t_2 + \delta$) are *similar*, so those two distributions can differ only by a phase factor independent of $\mathbf{r}_1 t_1$ and $\mathbf{r}_2 t_2$. Since when $t_2 \rightarrow t_1$ the first becomes $\delta(\mathbf{r}_2 - \mathbf{r}_1)$ and the second becomes $\delta(\mathbf{r}'_2 - \mathbf{r}'_1) (= \delta(\mathbf{r}_2 - \mathbf{r}_1))$ the phase factor can only be 1, so $\phi_{r_1}(\mathbf{r}_2 t_2) = \phi_{r_1 + \Delta, t_1 + \delta}(\mathbf{r}_2 + \Delta, t_2 + \delta)$ and the form (1.6) follows.

Use of the transformation group of system rotations:

Let us make a rotation ϕ of the spatial position vectors \mathbf{r}_1 and \mathbf{r}_2 about an axis $\hat{\mathbf{u}}$ passing through the origin of coordinates. By the isotropy of space and the similarity principle we have

$$\phi_{r'_1}(\mathbf{r}'_2 t_2) = \phi_{r_1}(\mathbf{r}_2 t_2) e^{i\alpha}$$

where \mathbf{r}'_1 and \mathbf{r}'_2 are \mathbf{r}_1 and \mathbf{r}_2 rotated by ϕ about $\hat{\mathbf{u}}$, and the phase α is independent of $\mathbf{r}_1 t_1$ and $\mathbf{r}_2 t_2$, and must in fact be zero on account of the case when \mathbf{r}_1 and \mathbf{r}_2 point in the same direction as $\hat{\mathbf{u}}$ and $\phi_{r'_1}(\mathbf{r}'_2 t_2)$ and $\phi_{r_1}(\mathbf{r}_2 t_2)$ are necessarily equal. This shows that

* i.e. occupation by the particle of the same position in fixed space at the same time

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$\phi_{r_{t_1}}(\mathbf{r}_2 t_2)$ is invariant on rotation of \mathbf{r}_1 and \mathbf{r}_2 together. Hence F in (1.6) is invariant on rotation of \mathbf{R} , and so we can write

$$\phi_{r_{t_1}}(\mathbf{r}_2 t_2) = F(|\mathbf{R}|, \tau) = c(|\mathbf{R}|, \tau) \exp i(b(|\mathbf{R}|, \tau)) \quad (1.8)$$

where c and b are real functions of $|\mathbf{R}|$ and τ , c being positive.

Requirements of dimensionality:

In (1.8) c must, by (1.3), have dimensions of length to the power -3 , and b must be dimensionless. The only natural constants we have available to meet these conditions are the particle mass m and the unit of action \hbar .^{*} From $|\mathbf{R}|$, τ , m and \hbar we can form only one dimensionless combination namely $\frac{mR^2}{\hbar\tau}$ so we must have

$$\phi_{r_{t_1}}(\mathbf{r}_2 t_2) = \left(\frac{\hbar}{m} \tau\right)^{-3/2} f\left(\frac{mR^2}{\hbar\tau}\right) \exp ig\left(\frac{mR^2}{\hbar\tau}\right)$$

where $\tau > 0$ since we are assuming $t_1 < t_2$, and f and g are real functions, f being positive. We can absorb f into g by expressing f as the exponential of a new function and allowing g to be complex. Hence

$$\phi_{r_{t_1}}(\mathbf{r}_2 t_2) = \left(\frac{\hbar}{m} \tau\right)^{-3/2} \exp ig\left(\frac{mR^2}{\hbar\tau}\right) \quad (1.9)$$

where g is now a complex function.

Proof of the linearity of the function g :

Instead of considering the particle motion in 3-D space we can consider the independent motions of the projections of the particle's position on the x , y and z axes of our (Cartesian) rest frame. The 3-D transformation functions are then given by the product of the three transformation functions belonging to the projections. For the projection on the x axis we seek the functions $\phi_{x_1 t_1}(x_2 t_2)$ and $\phi_{x_2 t_2}(x_1 t_1)$ in

$$\begin{aligned} \Phi(dx_2 t_2 | dx_1 t_1) &= \phi_{x_1 t_1}(x_2 t_2) \sqrt{dx_1} \sqrt{dx_2}, \\ \Phi(dx_1 t_1 | dx_2 t_2) &= \phi_{x_2 t_2}(x_1 t_1) \sqrt{dx_2} \sqrt{dx_1}, \text{ and} \end{aligned}$$

^{*} We assume that m and \hbar are the only physical parameters that could have any bearing on the free orbital motion of the particle.

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$$\phi_{x_2 t_2}(x_1 t_1) = (\phi_{x_1 t_1}(x_2 t_2))^* . \quad (1.10)$$

The transformation group of coordinate displacements in space and time give, in a manner similar to the 3-D case, the form

$$\phi_{x_1 t_1}(x_2 t_2) = F(x, \tau)$$

(like (1.6)), x standing for $x_2 - x_1$ and τ for $t_2 - t_1$.

The transformation group of rotations in 3-D space, now limited to a rotation through angle π about the y axis, leads to the requirement $\phi_{-x_1 t_1}(-x_2 t_2) = \phi_{x_1 t_1}(x_2 t_2)$ or $F(-x, \tau) = F(x, \tau)$. So $\phi_{x_1 t_1}(x_2 t_2) = F(|x|, \tau)$ or

$$\phi_{x_1 t_1}(x_2 t_2) = c(|x|, \tau) \exp ib(|x|, \tau)$$

(cf. (1.8)) where c and b are real functions (c being positive).

Requirements of dimensionality now give

$$\phi_{x_1 t_1}(x_2 t_2) = \left(\frac{\hbar}{m} \tau\right)^{-1/2} \exp if\left(\frac{mx^2}{\hbar \tau}\right)$$

(like (1.9)) where f is a complex function. Application of (1.10) gives $\phi_{x_2 t_2}(x_1 t_1)$.

The transformation functions $\phi_{y_1 t_1}(y_2 t_2)$ and $\phi_{z_1 t_1}(z_2 t_2)$ must be of the same form:

$$\phi_{y_1 t_1}(y_2 t_2) = \left(\frac{\hbar}{m} \tau\right)^{-1/2} \exp if\left(\frac{my^2}{\hbar \tau}\right),$$

$$\phi_{z_1 t_1}(z_2 t_2) = \left(\frac{\hbar}{m} \tau\right)^{-1/2} \exp if\left(\frac{mz^2}{\hbar \tau}\right)$$

where y stands for $y_2 - y_1$ and z stands for $z_2 - z_1$. This follows from the similarity principle and the fact that $\phi_{x_1 t_1}(x_2 t_2)$, $\phi_{y_1 t_1}(y_2 t_2)$ and $\phi_{z_1 t_1}(z_2 t_2)$ are all the same functions (i.e. $\delta(x_2 - x_1)$, $\delta(y_2 - y_1)$ and $\delta(z_2 - z_1)$) in the limit $t_2 \rightarrow t_1$.

By the product rule for wave functions (section 3.7 of Chapter I) we thus have

$$\phi_{r_1 t_1}(r_2 t_2) = \left(\frac{\hbar}{m} \tau\right)^{-3/2} \exp i\left(f\left(\frac{mx^2}{\hbar \tau}\right) + f\left(\frac{my^2}{\hbar \tau}\right) + f\left(\frac{mz^2}{\hbar \tau}\right)\right).$$

Comparing this with the form (1.9) for the same distribution worked out in 3-D space, we see that

$$g\left(\frac{mR^2}{\hbar \tau}\right) = f\left(\frac{mx^2}{\hbar \tau}\right) + f\left(\frac{my^2}{\hbar \tau}\right) + f\left(\frac{mz^2}{\hbar \tau}\right)$$

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where $R^2 = x^2 + y^2 + z^2$. This implies g is a linear function of its argument, i.e.

$$g\left(\frac{mR^2}{\hbar\tau}\right) = A \frac{m}{\hbar\tau} (x^2 + y^2 + z^2) + B$$

where A and B are complex numerical constants. Hence we arrive at

$$\phi_{r_1 t_1}(\mathbf{r}_2 t_2) = \left(\frac{\hbar}{m}\tau\right)^{-3/2} \exp i\left(A \frac{m}{\hbar\tau} (x^2 + y^2 + z^2) + B\right). \quad (1.11)$$

Satisfying the initial condition:

The initial condition requires

$$\lim_{\tau \rightarrow 0} \left(\frac{\hbar}{m}\tau\right)^{-1/2} \exp i\left(A \frac{m}{\hbar\tau} x^2 + \frac{1}{3}B\right) = \delta(x).$$

By *Corollary 1* of Representation 1 in Appendix B, this is indeed possible provided (B.8) and (B.3) hold, i.e. provided

$$\text{Im}(A) \geq 0 \quad (1.12)$$

and

$$\left(\frac{\hbar}{m}\tau\right)^{-1/2} \exp i\frac{1}{3}B = (i\pi)^{-1/2} \left(\frac{\hbar\tau}{mA}\right)^{-1/2} \quad (1.13)$$

where the power to one-half function is defined as in Appendix A. Hence (1.11) becomes

$$\phi_{r_1 t_1}(\mathbf{r}_2 t_2) = \left((i\pi)^{-1/2} \left(\frac{\hbar\tau}{mA}\right)^{-1/2}\right)^3 \exp iA \frac{m}{\hbar\tau} (x^2 + y^2 + z^2). \quad (1.14)$$

Orthonormal requirement:

The transformation functions $\Phi(d^3\mathbf{r}_2 t_2 | d^3\mathbf{r}_1 t_1)$ must be orthonormal, i.e.

$$\sum_{d^3\mathbf{r}_2} (\Phi(d^3\mathbf{r}_2 t_2 | d^3\mathbf{r}_1 t_1))^* \Phi(d^3\mathbf{r}_2 t_2 | d^3\mathbf{r}'_1 t_1) = \delta_{d^3\mathbf{r}_1, d^3\mathbf{r}'_1}.$$

Therefore, by the first of (1.3) the distribution in (1.14) must satisfy

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$$\int \phi_{r_1 t_1}^*(\mathbf{r}_2 t_2) \phi_{r_1 t_1}(\mathbf{r}_2 t_2) d^3 \mathbf{r}_2 = \delta(\mathbf{r}_1 - \mathbf{r}_1')$$

or $\phi_{x_1 t_1}(x_2 t_2)$ must satisfy

$$\int \phi_{x_1 t_1}^*(x_2 t_2) \phi_{x_1 t_1}(x_2 t_2) dx_2 = \delta(x_1 - x_1'). \quad (1.15)$$

Substituting the x component part of (1.14) in (1.15) gives the requirement

$$(\pi)^{-1} \left(\frac{\hbar \tau}{m|A|} \right)^{-1} \int_{-\infty}^{\infty} e^{i \frac{m}{\hbar \tau} (-A^* (x_2 - x_1)^2 + A (x_2 - x_1')^2)} dx_2 = \delta(x_1 - x_1'). \quad (1.16)$$

Using result (A.1) of Appendix A to evaluate the integral, (1.16) becomes

$$(\pi)^{-1} \left(\frac{\hbar \tau}{m|A|} \right)^{-1} \left(\frac{i\pi}{(A - A^*) \frac{m}{\hbar \tau}} \right)^{1/2} e^{-i \frac{m |A|^2}{\hbar \tau A - A^*} (x_1 - x_1')^2} = \delta(x_1 - x_1') \quad (1.17)$$

where the existence of the integral requires (see (A.2))

$$\text{Im}(A - A^*) > 0 \quad (\text{i.e. } \text{Im}(A) > 0). \quad (1.18)$$

By Representation 1 of Appendix B, we see (1.17) can be satisfied but only if we let $A - A^* \rightarrow 0$. We therefore have to make A real in (1.14) or rather regard A as real with an infinitesimal positive imaginary part (to satisfy (1.18)). Or, in (1.14), A should be considered to approach a real value α from a complex value $\alpha + i\delta$ with $\delta > 0$.

For this to work it is necessary that condition (B.3) is fulfilled, i.e. that

$$(\pi)^{-1} \left(\frac{\hbar \tau}{m|A|} \right)^{-1} \left(\frac{i\pi}{(A - A^*) \frac{m}{\hbar \tau}} \right)^{1/2} = (i\pi)^{-1/2} \left(\frac{A - A^* \hbar \tau}{-|A|^2 m} \right)^{-1/2} \quad (1.19)$$

We easily confirm that (1.19) is satisfied and therefore conclude from (1.14) that

$$\phi_{r_1 t_1}(\mathbf{r}_2 t_2) = \left(\frac{\pi i \hbar (t_2 - t_1)}{\alpha m} \right)^{-3/2} \exp i \left(\frac{\alpha m (\mathbf{r}_2 - \mathbf{r}_1)^2}{\hbar (t_2 - t_1)} \right) \quad (1.20)$$

where (because the cut for the power-one-half function is taken along the negative real axis) $i^{-3/2} = e^{-i3\pi/4}$ and only the real numerical constant α remains to be found.* The

* Since we are assuming that m is the only particle property that can affect the free orbital motion the same result (1.20) holds for a particle of any type, i.e. α is the same for all particles. Note that the result (1.20) is consistent with the principle of indifference (section 5.2 of Chapter I) as it should be. For under knowledge $\mathbf{r}_1 t_1$ and no knowledge regarding the velocity of the particle (other than this is never infinite)

transformation function $\phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)$ is given by the conjugate of the RHS of (1.20). Both transformation functions have been derived assuming $t_2 > t_1$. But if $t_2 < t_1$ $\phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)$ is given by the RHS of (1.20) with \mathbf{r}_1 and \mathbf{r}_2 and t_1 and t_2 interchanged, and $\phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$ is therefore given by the conjugate of this which is the same as in (1.20). Therefore (1.20) holds for $t_2 > t_1$ as well as for $t_2 < t_1$.

By (1.20) the modulus of $\phi_{\mathbf{r}_1}(\mathbf{r}_2 t_2)$ remains constant as $\mathbf{r}_2 \rightarrow \infty$, so the form of $\phi_{\mathbf{r}_1}(\mathbf{r}_2 t_2)$ seems to violate the law of continuous motion (that particles do not move infinitely fast). But we are contemplating ideal preparation of the particle to ensure it has a definite position at time t_1 . As we know, the acquisition of such knowledge almost certainly leads to an infinite force acting on the particle at time t_1 causing it to move at infinite speed. In practice of course we cannot achieve exact knowledge of the particle position at time t_1 and our distribution will only approximately be given by (1.20). But we need (1.20) as an expression of the ideal case for use in theoretical arguments. The ideal nature of (1.20) is evident from the fact that, on account of the factor $\sqrt{d^3 \mathbf{r}_1}$ in it, the wave function $\Phi(d^3 \mathbf{r}_2 t_2 | d^3 \mathbf{r}_1 t_1)$ (given by the first of (1.3)) is, even without the (expected) factor $\sqrt{d^3 \mathbf{r}_2}$, infinitesimal throughout all space.

2. Derivation of the Schrödinger equation for a free particle

However it comes about, any pure knowledge Y of the particle's motion may be represented by a probability distribution $\Phi(d^3 \mathbf{r}_1 t_1 | Y)$ over the propositions (the propositional basis) claiming the particle is in one or other of the many volume elements $d^3 \mathbf{r}_1$ at time t_1 during the motion; or equivalently by the wave function $\psi(\mathbf{r}_1 t_1)$ in

$$\Phi(d^3 \mathbf{r}_1 t_1 | Y) = \psi(\mathbf{r}_1 t_1) \sqrt{d^3 \mathbf{r}_1}$$

where \mathbf{r}_1 is the position coordinate of the volume element $d^3 \mathbf{r}_1$, and t_1 the time.

Alternatively our pure knowledge can be represented by another probability distribution relating to another time t_2 i.e. by

we are indifferent with regard to where it is at time t_2 so $|\phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)|^2$ should be independent of $\mathbf{r}_2 - \mathbf{r}_1$ and it is. And since there is a natural distance, namely $\sqrt{\hbar(t_2 - t_1)/m}$, enabling us to distinguish absolutely different distances from the known initial position \mathbf{r}_1 we are not *absolutely* indifferent with regard to particle position at time t_2 so $\angle \phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$ should not necessarily be independent of $\mathbf{r}_2 - \mathbf{r}_1$ and it is not. However we *are* unable to absolutely distinguish positions on the sphere $|\mathbf{r}_2 - \mathbf{r}_1| = \text{const.}$, so $\angle \phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$ should be constant over such a sphere, and it is.

IV. Derivation of the Schrödinger equation

$$\Phi(d^3\mathbf{r}_2t_2|Y) = \psi(\mathbf{r}_2t_2)\sqrt{d^3\mathbf{r}_2}$$

where \mathbf{r}_2 is the position coordinate of the volume element $d^3\mathbf{r}_2$, and t_2 the other time.

These two distributions are related by Feynman's law:

$$\Phi(d^3\mathbf{r}_2t_2|Y) = \sum_{d^3\mathbf{r}_1} \Phi(d^3\mathbf{r}_2t_2|d^3\mathbf{r}_1t_1)\Phi(d^3\mathbf{r}_1t_1|Y)$$

so the wave functions are related by

$$\psi(\mathbf{r}_2t_2) = \int K(\mathbf{r}_2t_2;\mathbf{r}_1t_1)\psi(\mathbf{r}_1t_1)d^3\mathbf{r}_1 \quad (2.1)$$

where the kernel is the position/position transformation function:

$$K(\mathbf{r}_2t_2;\mathbf{r}_1t_1) = \phi_{\mathbf{r}_1t_1}(\mathbf{r}_2t_2). \quad (2.2)$$

Of course this kernel contains an unknown constant α (see (1.20)). Later (in section 5 of Chapter VI) we will use the correspondence principle to fix this constant at $\frac{1}{2}$.

Now it is well known that (with $\alpha = \frac{1}{2}$) the kernel in (2.2) (given the form of $\phi_{\mathbf{r}_1t_1}(\mathbf{r}_2t_2)$ in (1.20)) satisfies the Schrödinger equation for a free particle. With α unspecified it will therefore satisfy the Schrödinger equation with \hbar replaced by $\hbar/2\alpha$, i.e. $K(\mathbf{r} t ;\mathbf{r}_1t_1)$ as given by (2.2) satisfies

$$-\frac{\hbar}{i} \frac{\partial K}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 K \cdot \frac{1}{2\alpha}. \quad (2.3)$$

Therefore, by (2.1) our wave function $\psi(\mathbf{r} t)$ also satisfies the Schrödinger equation with \hbar replaced by $\hbar/2\alpha$, i.e.

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi \cdot \frac{1}{2\alpha}. \quad (2.4)$$

So pending the evaluation of α , we have derived the Schrödinger equation for free particle motion. It must hold at all times during free motion of the particle under the pure knowledge Y .

In our interpretation, (2.4) is a logical consequence given the (complex valued) probability theory (as an extension of logic) and the little knowledge we have regarding the physics of free particle motion – the existence of particle mass (as the only relevant

particle property), the existence of one and only one fundamental unit (the unit of action \hbar), the homogeneity and isotropy of space and the homogeneity of time.*

From (2.1) we see that our probability density $\psi(\mathbf{r}_2 t_2)$ at \mathbf{r}_2 and at a time t_2 not much greater than t_1 depends only on our probability density $\psi(\mathbf{r}_1 t_1)$ at points \mathbf{r}_1 (at time t_1) not far from \mathbf{r}_2 i.e. within a distance

$$|\mathbf{r}_2 - \mathbf{r}_1| \approx \sqrt{\frac{\hbar(t_2 - t_1)}{|\alpha|m}}, \quad (2.5)$$

of \mathbf{r}_2 , because for $|\mathbf{r}_2 - \mathbf{r}_1|$ much greater than this the kernel in (2.1) rapidly oscillates (see the phase factor in (1.20)) so the contribution to the integral in (2.1) becomes small (at least for all ‘normal’ distributions $\psi(\mathbf{r}_1 t_1)$). This is in agreement with the law of continuous motion (that particles do not move infinitely fast) which implies that knowledge at time t_1 about particle position at places not close to \mathbf{r}_2 has less and less bearing on $\psi(\mathbf{r}_2 t_2)$ as t_2 becomes closer and closer to t_1 . Of course in the extreme limit $t_2 \rightarrow t_1$ the kernel becomes the delta function $\delta(\mathbf{r}_2 - \mathbf{r}_1)$.

The effective concentration of the kernel in (2.1) for small $t_2 - t_1$ is reflected in the form of the Schrödinger equation (2.4) where in a short period of time t to $t + dt$ the change in ψ is

$$d\psi = \frac{\partial\psi}{\partial t} dt = \frac{i\hbar}{2m} \frac{1}{2\alpha} \nabla^2 \psi dt$$

i.e. dependent only on *local* spatial derivatives of ψ at time t .

3. Derivation of the Schrödinger equation for a particle moving under the action of a scalar potential

A particle may move under the action of a scalar potential $V(\mathbf{r}, t)$. This potential has the units of energy and a particle at position \mathbf{r} at time t then has ‘potential energy’ $V(\mathbf{r}, t)$ which we know may have an effect on particle motion subject to the first law of potential action (section 3.2 of Chapter III). The mechanism of interaction between particle and potential is unknown. We know only that in the classical limit the particle should move according to Newton’s laws with $-\nabla V$ interpreted as the force on the particle. As we have said before, in quantum mechanics the potential is more fundamental than in classical mechanics. Whereas in classical mechanics $V(\mathbf{r}, t)$ is defined only to within an arbitrary additive constant, in quantum mechanics its absolute value has physical

* The derivation of (2.4) given here is formally similar to the derivation (using classical probability) of the diffusion equation for tiny particles in a fluid (see Appendix H).

significance (see end of section 3.1) so the potential $V(\mathbf{r},t) + k$ where k is a constant is not the same physically as the potential $V(\mathbf{r},t)$.

3.1 Position/position transformation functions in a uniform constant potential

Supposing a particle experiences a *uniform constant* potential, so $V(\mathbf{r},t) = V$ is independent of both \mathbf{r} and t , we seek the effect this knowledge has on our particle position/position transformation functions.

We may repeat the arguments of section 1 up to and including (1.8) because with $V(\mathbf{r},t)$ constant the particle still moves in a homogeneous and isotropic (fixed) space and a homogeneous time. We suppose for the time being (as we did in section 1) that $t_2 > t_1$ so that τ is positive.

Requirements of dimensionality:

When we come to the requirements of dimensionality however, in addition to \hbar (dimension ML^2/T) and m (dimension M) and of course $|R|$ (dimension L) and τ (dimension T) we have a new quantity at our disposal namely the potential V (dimension ML^2/T^2).

From $|R|, \tau, m, \hbar$ and V we can form just two independent dimensionless combinations, for example $\frac{mR^2}{\hbar\tau}$ and $\frac{V}{\hbar}\tau$. So in (1.8) we can put

$$c(|R|, \tau) = \left(\frac{\hbar}{m}\tau\right)^{-3/2} h\left(\frac{mR^2}{\hbar\tau}, \frac{V}{\hbar}\tau\right),$$

$$b(|R|, \tau) = g\left(\frac{mR^2}{\hbar\tau}, \frac{V}{\hbar}\tau\right)$$

where h and g are real functions, h being positive. Absorbing h into g by expressing h as e to the power of a real function of $\frac{mR^2}{\hbar\tau}$ and $\frac{V}{\hbar}\tau$ we therefore have

$$\phi_{r_1}(\mathbf{r}_2 t_2) = \left(\frac{\hbar}{m}\tau\right)^{-3/2} \exp ig\left(\frac{mR^2}{\hbar\tau}, \frac{V}{\hbar}\tau\right) \quad (3.1.1)$$

where g is now a *complex* function.

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Linearity of the function g with respect to its first variable:

If we work instead with each of the independent motions of the projections of particle position onto the Cartesian axes as in section 1, we come up with similar expressions for the 1-D component wave functions:

$$\left. \begin{aligned} \phi_{x_1} (x_2 t_2) &= \left(\frac{\hbar}{m} \tau\right)^{-1/2} \exp i f\left(\frac{mx^2}{\hbar \tau}, \frac{V}{\hbar} \tau\right) \\ \phi_{y_1} (y_2 t_2) &= \left(\frac{\hbar}{m} \tau\right)^{-1/2} \exp i f\left(\frac{my^2}{\hbar \tau}, \frac{V}{\hbar} \tau\right) \\ \phi_{z_1} (z_2 t_2) &= \left(\frac{\hbar}{m} \tau\right)^{-1/2} \exp i f\left(\frac{mz^2}{\hbar \tau}, \frac{V}{\hbar} \tau\right) \end{aligned} \right\}, \quad (3.1.2)$$

where $x = x_2 - x_1$, $y = y_2 - y_1$, $z = z_2 - z_1$ and f is some complex function which must again be the same in each case.

From (3.1.2) and the product rule for transformation functions we must have

$$\phi_{r_1} (\mathbf{r}_2 t_2) = \left(\frac{\hbar}{m} \tau\right)^{-3/2} \exp i \left(f\left(\frac{mx^2}{\hbar \tau}, \frac{V}{\hbar} \tau\right) + f\left(\frac{my^2}{\hbar \tau}, \frac{V}{\hbar} \tau\right) + f\left(\frac{mz^2}{\hbar \tau}, \frac{V}{\hbar} \tau\right) \right). \quad (3.1.3)$$

Since the RHS of (3.1.1) must equal that of (3.1.3) for all τ, x^2, y^2 and z^2 (R^2 being equal to $x^2 + y^2 + z^2$ in (3.1.1)) it can only be that g is linear in its first variable*, i.e.

$$g\left(\frac{mR^2}{\hbar \tau}, \frac{V}{\hbar} \tau\right) = A\left(\frac{V}{\hbar} \tau\right) \frac{m}{\hbar \tau} (x^2 + y^2 + z^2) + B\left(\frac{V}{\hbar} \tau\right) \quad (3.1.4)$$

with

$$f\left(\frac{mx^2}{\hbar \tau}, \frac{V}{\hbar} \tau\right) = A\left(\frac{V}{\hbar} \tau\right) \frac{mx^2}{\hbar \tau} + \frac{1}{3} B\left(\frac{V}{\hbar} \tau\right). \quad (3.1.5)$$

Using (3.1.4) and (3.1.1) gives

$$\phi_{r_1} (\mathbf{r}_2 t_2) = \left(\frac{\hbar}{m} \tau\right)^{-3/2} \exp i \left(A\left(\frac{V}{\hbar} \tau\right) \frac{m}{\hbar \tau} (x^2 + y^2 + z^2) + B\left(\frac{V}{\hbar} \tau\right) \right) \quad (3.1.6)$$

which differs from the zero potential result (1.11) in that A and B may now be complex functions of $\frac{V}{\hbar} \tau$ rather than complex constants.

* For in general if $g(x + y + z) = f(x) + f(y) + f(z)$ we have after differentiation with respect to x that $g'(x + y + z) = f'(x)$ showing g' can only be constant.

IV. Derivation of the Schrödinger equation

Consistency with Feynman's law:

From (3.1.2) and (3.1.5) the position/position transformation function for the projection of particle position onto the x axis of Cartesian coordinates is

$$\phi_{x_1 t_1}(x_2 t_2) = \left(\frac{\hbar}{m}(t_2 - t_1)\right)^{-1/2} \exp i \left(A \left(\frac{V}{\hbar}(t_2 - t_1) \right) \frac{m(x_2 - x_1)^2}{\hbar(t_2 - t_1)} + \frac{1}{3} B \left(\frac{V}{\hbar}(t_2 - t_1) \right) \right) \quad (3.1.7)$$

where A and B are complex functions and $t_2 > t_1$.

If x_3 is the position at time $t_3 (> t_2)$ we have similarly

$$\phi_{x_2 t_2}(x_3 t_3) = \left(\frac{\hbar}{m}(t_3 - t_2)\right)^{-1/2} \exp i \left(A \left(\frac{V}{\hbar}(t_3 - t_2) \right) \frac{m(x_3 - x_2)^2}{\hbar(t_3 - t_2)} + \frac{1}{3} B \left(\frac{V}{\hbar}(t_3 - t_2) \right) \right) \quad (3.1.8)$$

and

$$\phi_{x_1 t_1}(x_3 t_3) = \left(\frac{\hbar}{m}(t_3 - t_1)\right)^{-1/2} \exp i \left(A \left(\frac{V}{\hbar}(t_3 - t_1) \right) \frac{m(x_3 - x_1)^2}{\hbar(t_3 - t_1)} + \frac{1}{3} B \left(\frac{V}{\hbar}(t_3 - t_1) \right) \right) \quad (3.1.9)$$

But distributions $\phi_{x_1 t_1}(x_3 t_3)$ and $\phi_{x_1 t_1}(x_2 t_2)$ are alternative representations of the same state of knowledge. They must therefore be related by Feynman's law thus

$$\phi_{x_1 t_1}(x_3 t_3) = \int_{-\infty}^{\infty} \phi_{x_2 t_2}(x_3 t_3) \phi_{x_1 t_1}(x_2 t_2) dx_2 \quad (3.1.10)$$

This imposes a condition on the unknowns in (3.1.6). Substituting the expressions (3.1.7) to (3.1.8) for the wave functions and the RHS of (3.1.10) we obtain an integral of a form

$$\int_{-\infty}^{\infty} e^{i\alpha(x_2 - x_1)^2 + i\beta(x_3 - x_2)^2} dx_2$$

where

$$\alpha = A \left(\frac{V}{\hbar}(t_2 - t_1) \right) \frac{m}{\hbar(t_2 - t_1)}, \quad \beta = A \left(\frac{V}{\hbar}(t_3 - t_2) \right) \frac{m}{\hbar(t_3 - t_2)}. \quad (3.1.11)$$

According to Appendix A, the integral exists only when $\text{Im}(\alpha + \beta) \geq 0$ and then

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$$\int_{-\infty}^{\infty} e^{i\alpha(x_2-x_1)^2+i\beta(x_3-x_2)^2} dx_2 = \left(\frac{i\pi}{\alpha+\beta}\right)^{\frac{1}{2}} e^{\frac{i\alpha\beta}{\alpha+\beta}(x_3-x_1)^2}, \quad (3.1.12)$$

where the power one-half function is defined in Appendix A. Using this result we find that (3.1.10) requires

$$\begin{aligned} & \left(\frac{\hbar}{m}(t_3-t_1)\right)^{-1/2} \exp i\left(A\left(\frac{V}{\hbar}(t_3-t_1)\right)\frac{m(x_3-x_1)^2}{\hbar(t_3-t_1)} + \frac{1}{3}B\left(\frac{V}{\hbar}(t_3-t_1)\right)\right) = \\ & \left(\frac{\hbar}{m}(t_2-t_1)\right)^{-1/2} \exp i\left(\frac{1}{3}B\left(\frac{V}{\hbar}(t_2-t_1)\right)\right) \cdot \left(\frac{\hbar}{m}(t_3-t_2)\right)^{-1/2} \exp i\left(\frac{1}{3}B\left(\frac{V}{\hbar}(t_3-t_2)\right)\right) \cdot \left(\frac{i\pi}{\alpha+\beta}\right)^{\frac{1}{2}} e^{\frac{i\alpha\beta}{\alpha+\beta}(x_3-x_1)^2} \\ & \dots(3.1.13) \end{aligned}$$

We may equate the coefficients multiplying $(x_3-x_1)^2$ in the exponents in (3.1.13)* giving

$$A\left(\frac{V}{\hbar}(t_3-t_1)\right)\frac{m}{\hbar(t_3-t_1)} = \frac{\alpha\beta}{\alpha+\beta} = \frac{A\left(\frac{V}{\hbar}(t_2-t_1)\right)\frac{m}{\hbar(t_2-t_1)}A\left(\frac{V}{\hbar}(t_3-t_2)\right)\frac{m}{\hbar(t_3-t_2)}}{A\left(\frac{V}{\hbar}(t_2-t_1)\right)\frac{m}{\hbar(t_2-t_1)} + A\left(\frac{V}{\hbar}(t_3-t_2)\right)\frac{m}{\hbar(t_3-t_2)}}.$$

Considering the special case in which $t_3-t_2=t_2-t_1=\tau$ (so that $t_3-t_1=2\tau$) this gives

$$A\left(\frac{V}{\hbar}2\tau\right) = A\left(\frac{V}{\hbar}\tau\right)$$

for all τ , proving that A must be a constant.

In (3.1.13) $\alpha+\beta$ is, from (3.1.11), given by

$$\alpha+\beta = A\frac{m}{\hbar}\left(\frac{1}{(t_2-t_1)} + \frac{1}{(t_3-t_2)}\right) = A\frac{m}{\hbar}\frac{(t_3-t_1)}{(t_2-t_1)(t_3-t_2)}$$

so (3.1.13) simplifies to

$$\exp i\left(\frac{1}{3}B\left(\frac{V}{\hbar}(t_3-t_1)\right)\right) = \left(\frac{i\pi}{A}\right)^{1/2} \exp i\left(\frac{1}{3}B\left(\frac{V}{\hbar}(t_2-t_1)\right) + \frac{1}{3}B\left(\frac{V}{\hbar}(t_3-t_2)\right)\right).$$

* If the coefficients are denoted P and Q , (3.1.13) can be written $e^{i(P-Q)(x_3-x_1)^2} = K$ where K is independent of (x_3-x_1) . It follows that $P-Q$ can only be zero.

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Writing $A = A_0 e^{i\alpha_0}$, where $-\pi < \frac{\pi}{2} - \alpha_0 \leq \pi$ and $A_0 > 0$, this gives

$$B\left(\frac{V}{\hbar}(t_3 - t_1)\right) = B\left(\frac{V}{\hbar}(t_2 - t_1)\right) + B\left(\frac{V}{\hbar}(t_3 - t_2)\right) + 3\left(\frac{\pi}{4} - \frac{\alpha_0}{2}\right) - 3i \ln\left(\sqrt{\frac{\pi}{A_0}}\right) \quad (3.1.14)$$

showing B can only be a linear function of its argument, i.e.

$$B(z) = \gamma z + \delta$$

with

$$\delta = -3\left(\frac{\pi}{4} - \frac{\alpha_0}{2}\right) + 3i \ln\sqrt{\frac{\pi}{A_0}}.$$

Hence $\phi_{x_1 t_1}(x_2 t_2)$ in (3.1.7) must in fact be of the form

$$\phi_{x_1 t_1}(x_2 t_2) = \left(\frac{\hbar}{m}(t_2 - t_1)\right)^{-1/2} \exp i\left(A \frac{m(x_2 - x_1)^2}{\hbar(t_2 - t_1)} + \frac{1}{3}\gamma \frac{V}{\hbar}(t_2 - t_1) - \left(\frac{\pi}{4} - \frac{\alpha_0}{2}\right) + i \ln\sqrt{\frac{\pi}{A_0}}\right)$$

or since

$$\exp i\left(-\left(\frac{\pi}{4} - \frac{\alpha_0}{2}\right) + i \ln\sqrt{\frac{\pi}{A_0}}\right) = \left(\frac{i\pi}{A}\right)^{-1/2}$$

we must have

$$\phi_{x_1 t_1}(x_2 t_2) = \left(\frac{i\pi\hbar}{Am}(t_2 - t_1)\right)^{-1/2} \exp i\left(A \frac{m(x_2 - x_1)^2}{\hbar(t_2 - t_1)} + \frac{1}{3}\gamma \frac{V}{\hbar}(t_2 - t_1)\right)$$

where A and γ are numerical constants. This must hold for all $x_2 t_2$, $x_1 t_1$ and V . So, putting $V = 0$ we see that A must be the same as the *real* constant α in (1.20). Also γ must be real otherwise the orthonormal requirement (1.15) would not be satisfied when V was different from zero.

By forming the product of the transformation functions for each projection, we arrive at the result

$$\phi_{r_1 t_1}(\mathbf{r}_2 t_2) = \left(\frac{i\pi\hbar}{\alpha m}(t_2 - t_1)\right)^{-3/2} \exp i\left(\frac{\alpha m(\mathbf{r}_2 - \mathbf{r}_1)^2}{\hbar(t_2 - t_1)} + \gamma \frac{V}{\hbar}(t_2 - t_1)\right) \quad (3.1.15)$$

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where α and γ are real numerical constants yet to be found.* The transformation function $\phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)$ is of course the conjugate of that in (3.1.15). And, for the same reasons as we noted in connection with result (1.20), the result (3.1.15) holds whether t_2 is greater than or less than t_1 .

Assuming $\gamma \neq 0$ (and in section 5 of Chapter VI we will find that γ is necessarily equal to -1) the form of (3.1.15) shows that motion of a particle in a constant uniform (non-zero) potential proceeds differently from the case of zero potential. Otherwise, (having calculable absolute phases) the transformation functions for $V = 0$ and for $V \neq 0$ would (by the similarity principle) have to be identical at any time t_2 .

3.2 Schrödinger equation for a particle moving under the action of a potential

The Schrödinger equation for a *constant uniform* potential can be derived in the same way as for a free particle (section 2). Equation (2.1) remains valid but now the kernel in (2.2) is given by (3.1.15) i.e. it now includes the factor

$$\exp i\left(\gamma \frac{V}{\hbar}(t_2 - t_1)\right).$$

So instead of satisfying (2.3), the kernel $K(\mathbf{r} t ; \mathbf{r}_1 t_1)$ in the case of a constant uniform potential satisfies

$$-\frac{\hbar}{i} \frac{\partial K}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 K - \frac{1}{2\alpha} K - \gamma V K. \quad (3.2.1)$$

And accordingly, under pure knowledge Y , our wave function $\psi(\mathbf{r} t)$ satisfies

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{1}{2\alpha} \psi - \gamma V \psi. \quad (3.2.2)$$

The point noted (at the end of section 2) about the effective concentration of the kernel $K(\mathbf{r}_2 t_2 ; \mathbf{r}_1 t_1)$ within a distance (2.5) for small time intervals $t_2 - t_1$, remains mathematically valid in the case of the kernel for a particle in a constant uniform potential field.

This is again reflected in the Schrödinger equation (3.2.2) where at any point in space the change in ψ in a short time depends only on the local values of $\nabla^2 \psi$, ψ and V . By (3.2.2), after a short time dt the value of $\psi(\mathbf{r}, t)$ changes thus:

* We are assuming particle mass m and particle potential energy V are the only particle properties affecting the particle motion. This means γ as well as α is independent of particle type. (See footnote following (1.20).)

$$\psi \rightarrow \psi + \frac{-i}{\hbar} \left(-\frac{\hbar^2}{2m} \nabla^2 \psi \frac{1}{2\alpha} - \gamma V \psi \right) dt. \quad (3.2.3)$$

The Schrödinger equation for a particle in a general *variable* and *non-uniform* potential field $V(\mathbf{r}, t)$ can be derived as follows. Suppose we hold pure knowledge Y relating to the particle motion from which we can infer that a particular wave function $\psi(\mathbf{r}, t)$ applies at time t . Suppose knowing $\psi(\mathbf{r}, t)$ everywhere at time t we set ourselves the problem of calculating $\psi(\mathbf{r}, t)$ inside a small volume element dV any short time dt later. For this purpose we form the sample space S'_t of propositions regarding particle motion from time t onwards. Let dV' be a small volume element enclosing dV .

We know, from the first law of potential action, that the motion of the particle between times t and $t+dt$, should it be in dV at that time, is affected by the value of the potential $V(\mathbf{r}, t)$ in dV' , but not by the spatial or temporal derivatives of $V(\mathbf{r}, t)$ in dV' nor by the potential $V(\mathbf{r}, t)$ outside dV' between times t and $t+dt$ nor by $V(\mathbf{r}, t)$ anywhere at future times. It may be affected by the potential $V(\mathbf{r}, t)$ at positions the particle may have occupied at *earlier* times, but since we have pure knowledge Y in S'_t (expressed by $\psi(\mathbf{r}, t)$ at time t), knowledge of $V(\mathbf{r}, t)$ at earlier times is redundant (see section 3.2 of Chapter I).*

We know that the particle does not move infinitely fast so that our knowledge $\psi(\mathbf{r}, t)$ regarding particle position at time t for \mathbf{r} outside the small volume element dV' enclosing dV is, for our purpose, superfluous. Therefore our problem is *similar* to the one in which the potential is (from time t to time $t+dt$) constant in time and space and equal to the local value of $V(\mathbf{r}, t)$ at the position of dV and at the time t in question. In that case (3.2.3) holds for the change in $\psi(\mathbf{r}, t)$ over any short enough time. So by the similarity principle, for \mathbf{r} in dV and after any short time dt

$$\psi(\mathbf{r}, t+dt) = \left(\psi(\mathbf{r}, t) + \frac{-i}{\hbar} \left(-\frac{\hbar^2}{2m} \nabla^2 \psi \frac{1}{2\alpha} - \gamma V(\mathbf{r}, t) \psi \right) dt \right) e^{i\beta} \quad (3.2.4)$$

where β is a real constant independent of dt . But for $dt \rightarrow 0$ we must have $\psi(\mathbf{r}, t+dt) = \psi(\mathbf{r}, t)$ so that β can only be zero and $\psi(\mathbf{r}, t)$ must satisfy

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi \frac{1}{2\alpha} - \gamma V(\mathbf{r}, t) \psi \quad (3.2.5)$$

in any short enough time interval. Being valid for any short enough time interval, and in any volume element dV , (3.2.5) is valid for all times and positions in space and (except

* It is still quite possible that the motion after time t is dependent on $V(\mathbf{r}, t)$ at earlier times. It is just that we do not need to involve earlier values of $V(\mathbf{r}, t)$ in our present logical argument. The effect of $V(\mathbf{r}, t)$ at earlier times is if you like already incorporated in the form of the wave function $\psi(\mathbf{r}, t)$ at time t .

for the values of the numerical constants α and γ) we have established the Schrödinger equation for a particle moving under the action of a general scalar potential.*

In section 5 we will establish the relation $\gamma = -2\alpha$ between γ and α . The correct numerical value of α (namely $\alpha = \frac{1}{2}$) will be established in section 5 of Chapter VI.

4. Case of particle motion under the action of a vector potential

The derivation of the Schrödinger equation in the case of a *vector* potential (or of a combination of vector and scalar potentials) proceeds in a very similar way to the case of a scalar potential. We suppose both kinds of potential are present and start by finding the transformation function $\phi_{r_1 t_1}(r_2 t_2)$ when the potentials are constant in space and time.

4.1 Position/position transformation functions in uniform constant vector and scalar potentials

The homogeneity of space and time again leads to the form

$$\phi_{r_1 t_1}(r_2 t_2) = F(\mathbf{R}, \tau). \quad (4.1.1)$$

as in (1.6) but now rotational invariance is present only for rotations of \mathbf{R} about an axis parallel to \mathbf{A} . This means we can write[†]

$$\phi_{r_1 t_1}(r_2 t_2) = F(|\mathbf{R}|, \mathbf{A} \cdot \mathbf{R}, |\mathbf{A}|, \tau) \quad (4.1.2)$$

and for now we assume (again) that $\tau > 0$. We have in (4.1.2) the form of $\phi_{r_1 t_1}(r_2 t_2)$ as a function of \mathbf{R} , \mathbf{A} and τ , but in (4.1.2), F may of course also depend separately on V .

* In the usual formulation of quantum mechanics Schrödinger's equation (3.2.5) is often viewed as a fundamental law of motion, giving the evolution of the state of the system and becoming Newton's second law of motion when $\psi(\mathbf{r}, t)$ is a small wave packet and $V(\mathbf{r}, t)$ is slowly changing in space and time. It may therefore seem strange that we are apparently able to derive it from general physical assumptions like the homogeneity of space and time. But we claim only that $\psi(\mathbf{r}, t)$ represents an evolving *probability distribution* not the evolving *state* of the system. Thus (3.2.5) relates only to our rational degrees of belief regarding particle position at various times given our limited knowledge. It gives, in repeated trials and at any one time, expected frequencies of occupation by the particle of volume elements of space; but expected frequencies are not actual frequencies (see Appendix F) and in small wave packet cases $\psi(\mathbf{r}, t)$ is not zero outside or even far away from the packet, so (3.2.5) in fact leaves open the possibility of any actual motion of the particle. It is not a law of motion.

† Taking \mathbf{R} and \mathbf{A} to originate from the origin of abstract 3-D space, F must be constant as \mathbf{R} rotates about \mathbf{A} . Only the configuration of \mathbf{R} in relation to \mathbf{A} in a plane containing \mathbf{R} and \mathbf{A} matters. This configuration is evidently fixed by specifying $|\mathbf{R}|$, $|\mathbf{A}|$ and the angle θ between \mathbf{R} and \mathbf{A} , or rather the cosine of that angle, (θ and $-\theta$ being equivalent). Hence the form (4.1.2).

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There are only four independent dimensionless combinations of $|\mathbf{R}|, \mathbf{A}\cdot\mathbf{R}, |\mathbf{A}|, \tau, V, m$ and \hbar , for example $\frac{mR^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}\mathbf{A}\cdot\mathbf{R}$ and $\frac{A^2\tau}{m\hbar}$, where $R^2 = |\mathbf{R}|^2, A^2 = |\mathbf{A}|^2$. Hence we can write

$$\phi_{r_1 t_1}(r_2 t_2) = \left(\frac{\hbar}{m}\tau\right)^{-3/2} \exp ig\left(\frac{mR^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}\mathbf{A}\cdot\mathbf{R}, \frac{A^2\tau}{m\hbar}\right) \quad (4.1.3)$$

in place of (3.1.1).

The separate x, y and z Cartesian components of the motion take place under constant 1-D vector potentials A_x, A_y and A_z respectively.

In place of (4.1.1) and for the same reason, we can write for the x component transformation function

$$\phi_{x_1 t_1}(x_2 t_2) = F(x, \tau)$$

where $x = x_2 - x_1, \tau = t_2 - t_1$.

Using the law of inversion and the similarity principle we obtain the relation

$$\phi_{-x_1 t_1 - A_x}(-x_2 t_2) = \phi_{x_1 t_1 A_x}(x_2 t_2) \quad (4.1.4)$$

where dependence of the transformation function on A_x is made explicit. This is because for every motion of the projection of the particle on the x axis there is an inverted motion (see section 3.11 of Chapter III) with the component A_x of \mathbf{A} also inverted. So the similarity principle gives (4.1.4) with a phase factor $e^{i\alpha}$ on the RHS independent of $x_1 t_1, x_2 t_2$ and A_x . The phase α must however be zero because when $x_1 = x_2 = 0$ and $A_x = 0$ both sides of (4.1.4) are for certain the same.

It follows from (4.1.4) that as a function of x, A_x and τ, F must have the form* $F(|x|, A_x x, |A_x|, \tau)$, i.e.

$$\phi_{x_1 t_1}(x_2 t_2) = F(|x|, A_x x, |A_x|, \tau)$$

in place of (4.1.2). F might of course depend also on V (as well as on \hbar and m).

There are only three independent dimensionless combinations of $|x|, A_x x, |A_x|, \tau, V, m$, and \hbar , for example, $mx^2/\hbar\tau$ are $V\tau/\hbar$ and $A_x x/\hbar$, hence we can write

* F can depend only on the configuration of the 1-D vectors x and A_x i.e. on $|x|$ and $|A_x|$ and on the relative signs of x and A_x or on the sign of $A_x x$.

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$$\left. \begin{aligned} \phi_{x_1 t_1}(x_2 t_2) &= \left(\frac{\hbar}{m}\tau\right)^{-1/2} \exp if\left(\frac{mx^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}A_x x\right) \\ \phi_{y_1 t_1}(y_2 t_2) &= \left(\frac{\hbar}{m}\tau\right)^{-1/2} \exp if\left(\frac{my^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}A_y y\right) \\ \phi_{z_1 t_1}(z_2 t_2) &= \left(\frac{\hbar}{m}\tau\right)^{-1/2} \exp if\left(\frac{mz^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}A_z z\right) \end{aligned} \right\} \quad (4.1.5)$$

in place of (3.1.2). The product of these must return us to $\phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$ in (4.1.3), giving us the identity

$$\begin{aligned} &f\left(\frac{mx^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}A_x x\right) + f\left(\frac{my^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}A_y y\right) + f\left(\frac{mz^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}A_z z\right) = \\ &g\left(\frac{m(x^2 + y^2 + z^2)}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}(A_x x + A_y y + A_z z), \frac{(A_x^2 + A_y^2 + A_z^2)\tau}{m\hbar}\right) \end{aligned}$$

which shows $g\left(\frac{mR^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}\mathbf{A}\cdot\mathbf{R}, \frac{A^2\tau}{m\hbar}\right)$ must be a linear function of its first, third and fourth variables.* So in place of (3.1.4) and (3.1.5) we have

$$g = \bar{A}\left(\frac{V}{\hbar}\tau\right)\frac{mR^2}{\hbar\tau} + \bar{C}\left(\frac{V}{\hbar}\tau\right)\frac{1}{\hbar}\mathbf{A}\cdot\mathbf{R} + \bar{D}\left(\frac{V}{\hbar}\tau\right)\frac{A^2\tau}{m\hbar} + \bar{B}\left(\frac{V}{\hbar}\tau\right) \quad (4.1.6)$$

and

* Thinking of f and g as functions of x, y, z and A_x, A_y, A_z (and numbering some equations (1), (2), ... etc.) we have

$$f(x^2, ax) + f(y^2, by) + f(z^2, cz) = g(x^2 + y^2 + z^2, ax + by + cz, a^2 + b^2 + c^2) \quad (1)$$

where a, b, c stand for A_x, A_y, A_z . Putting $y = z = 0$ and differentiating with respect to b we get

$$h'(b) = g_3(x^2, ax, a^2 + b^2 + c^2)2b \quad (2), \text{ where we suppose } f(y^2, by) \rightarrow h(b) \text{ as } y \rightarrow 0. \text{ This}$$

shows (by independent variation of the variables in g_3 - the first derivative of g with respect to its third variable) that g_3 is a constant (say B), making g equal to B times its third variable plus a function of

its first and second variables, and $h(b) = Bb^2 + k \quad (3)$, where k is a constant. Replacing, as we may, the

f functions in (1) by functions of a^2 and ax etc rather than x^2 and ax etc we can show similarly that g is a constant (say A) times its first variable plus a function of its second and third variables. Hence

$$g(x^2, ax, a^2 + b^2 + c^2) = Ax^2 + B(a^2 + b^2 + c^2) + F(ax) \quad (4), \text{ where } F \text{ is some function. So by}$$

(3), and by putting $y = z = 0$, (1) gives $f(x^2, ax) = Ax^2 + Ba^2 + F(ax) - 2k \quad (5)$. Using forms (4)

and (5) for g and f , (1) now gives $F(ax + by + cz) = F(ax) + F(by) + F(cz) - 6k$ showing F is a linear function. Hence g in (1) is linear in all three of its variables.

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$$f\left(\frac{mx^2}{\hbar\tau}, \frac{V}{\hbar}\tau, \frac{1}{\hbar}A_x x\right) = \bar{A}\left(\frac{V}{\hbar}\tau\right)\frac{mx^2}{\hbar\tau} + \bar{C}\left(\frac{V}{\hbar}\tau\right)\frac{1}{\hbar}A_x x + \bar{D}\left(\frac{V}{\hbar}\tau\right)\frac{A_x^2\tau}{m\hbar} + \frac{1}{3}\bar{B}\left(\frac{V}{\hbar}\tau\right) \quad (4.1.7)$$

where $\bar{A}, \bar{B}, \bar{C}$ and \bar{D} are functions of $V\tau/\hbar$ only.

Hence in (3.1.10) we should now put

$$\left. \begin{aligned} \phi_{x_1 t_1}(x_3 t_3) &= \left(\frac{\hbar}{m}(t_3 - t_1)\right)^{-1/2} \exp i(\bar{\beta}(x_3 - x_1)^2 + \bar{\varepsilon}(x_3 - x_1) + \frac{1}{3}\bar{\alpha}(t_3 - t_1)) \\ \phi_{x_2 t_2}(x_3 t_3) &= \left(\frac{\hbar}{m}(t_3 - t_2)\right)^{-1/2} \exp i(\beta(x_3 - x_2)^2 + \varepsilon(x_3 - x_2) + \frac{1}{3}\bar{\alpha}(t_3 - t_2)) \\ \phi_{x_1 t_1}(x_2 t_2) &= \left(\frac{\hbar}{m}(t_2 - t_1)\right)^{-1/2} \exp i(\alpha(x_2 - x_1)^2 + \gamma(x_2 - x_1) + \frac{1}{3}\bar{\alpha}(t_2 - t_1)) \end{aligned} \right\} \quad (4.1.8)$$

where the coefficients $\bar{\beta}, \bar{\varepsilon}, \beta, \varepsilon, \alpha$ and γ , and the function $\bar{\alpha}$ are

$$\left. \begin{aligned} \bar{\beta} &= \bar{A}\left(\frac{V}{\hbar}(t_3 - t_1)\right)\frac{m}{\hbar(t_3 - t_1)}, & \bar{\varepsilon} &= \bar{C}\left(\frac{V}{\hbar}(t_3 - t_1)\right)\frac{A_x}{\hbar} \\ \beta &= \bar{A}\left(\frac{V}{\hbar}(t_3 - t_2)\right)\frac{m}{\hbar(t_3 - t_2)}, & \varepsilon &= \bar{C}\left(\frac{V}{\hbar}(t_3 - t_2)\right)\frac{A_x}{\hbar} \\ \alpha &= \bar{A}\left(\frac{V}{\hbar}(t_2 - t_1)\right)\frac{m}{\hbar(t_2 - t_1)}, & \gamma &= \bar{C}\left(\frac{V}{\hbar}(t_2 - t_1)\right)\frac{A_x}{\hbar} \\ \bar{\alpha}(\tau) &= 3\bar{D}\left(\frac{V}{\hbar}\tau\right)\frac{A_x^2\tau}{m\hbar} + \bar{B}\left(\frac{V}{\hbar}\tau\right) \end{aligned} \right\} \quad (4.1.9)$$

where τ is $t_3 - t_1$, $t_3 - t_2$ or $t_2 - t_1$.

Since coefficients $\bar{\beta}, \beta$ and α in (4.1.8) are (by (4.1.9)) independent of A_x they remain unchanged as $A_x \rightarrow 0$ and must equal the corresponding factors in (3.1.9), (3.1.8) and (3.1.7), i.e. \bar{A} is the same function as A in section 3.1. Similarly the part \bar{B} of $\bar{\alpha}$ in the last of (4.1.9) is independent of A_x and remains unchanged as $A_x \rightarrow 0$, so \bar{B} is the same function as B in section 3.1.

Using the result

$$\int_{-\infty}^{\infty} e^{i\alpha(x_2 - x_1)^2 + i\beta(x_3 - x_2)^2 + i\gamma(x_2 - x_1) + i\varepsilon(x_3 - x_2)} dx_2 = \left(\frac{i\pi}{\alpha + \beta}\right)^{1/2} e^{i\left(\frac{\alpha\beta}{\alpha + \beta}(x_3 - x_1)^2 + \frac{(\alpha\varepsilon + \beta\gamma)}{\alpha + \beta}(x_3 - x_1) - \frac{1}{4}\frac{(\gamma - \varepsilon)^2}{\alpha + \beta}\right)}$$

of Appendix A (where conditions for the existence of the integral are given) we obtain from (3.1.10) and (4.1.8) the result

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$$\begin{aligned}
& \left(\frac{\hbar}{m}(t_3-t_1)\right)^{-1/2} \exp i(\bar{\beta}(x_3-x_1)^2 + \bar{\varepsilon}(x_3-x_1) + \frac{1}{3}\bar{\alpha}(t_3-t_1)) \\
&= \left(\frac{\hbar}{m}(t_3-t_2)\right)^{-1/2} \left(\frac{\hbar}{m}(t_2-t_1)\right)^{-1/2} \exp i\frac{1}{3}(\bar{\alpha}(t_3-t_2) + \bar{\alpha}(t_2-t_1)) \\
& \left(\frac{i\pi}{\alpha+\beta}\right)^{1/2} \exp i\left(\frac{\alpha\beta}{\alpha+\beta}(x_3-x_1)^2 + \frac{\alpha\varepsilon+\beta\gamma}{\alpha+\beta}(x_3-x_1) - \frac{1}{4}\frac{(\gamma-\varepsilon)^2}{\alpha+\beta}\right).
\end{aligned} \tag{4.1.10}$$

As in the case of (3.1.13) we may equate the coefficients multiplying $(x_3-x_1)^2$ and (now also) the coefficients multiplying (x_3-x_1) in the exponents on the LHS and RHS of (4.1.10). This gives

$$\bar{\beta} = \frac{\alpha\beta}{\alpha+\beta}, \quad \bar{\varepsilon} = \frac{\alpha\varepsilon+\beta\gamma}{\alpha+\beta} \tag{4.1.11}$$

and cancelling out the exponent terms in $(x_3-x_1)^2$ and (x_3-x_1) , (4.1.10) reduces to

$$\begin{aligned}
& \left(\frac{\hbar}{m}(t_3-t_1)\right)^{-1/2} \exp i\frac{1}{3}\bar{\alpha}(t_3-t_1) \\
&= \left(\frac{\hbar}{m}(t_3-t_2)\right)^{-1/2} \left(\frac{\hbar}{m}(t_2-t_1)\right)^{-1/2} \exp i\frac{1}{3}(\bar{\alpha}(t_3-t_2) + \bar{\alpha}(t_2-t_1)) \\
& \left(\frac{i\pi}{\alpha+\beta}\right)^{1/2} \exp i\left(-\frac{1}{4}\frac{(\gamma-\varepsilon)^2}{\alpha+\beta}\right).
\end{aligned} \tag{4.1.12}$$

Substituting in (4.1.11) for $\bar{\beta}, \bar{\varepsilon}, \beta, \varepsilon, \alpha, \gamma$ as given in (4.1.9), the first of (4.1.11) shows \bar{A} must be constant (for the same reason that A had to be constant in section 3.1). In a similar manner the second of (4.1.11) shows \bar{C} must be constant. Hence $\gamma-\varepsilon$ is zero and (4.1.12) reduces to the same equation for the function $\bar{\alpha}(\tau)$ (involving $\bar{A} (= \bar{A}_0 e^{i\bar{\alpha}_0})$) as (3.1.13) gave (in (3.1.14)) for the function $B(\frac{V}{\hbar}\tau)$ (involving $A (= A_0 e^{i\alpha_0})$), i.e.

$$\bar{\alpha}(t_3-t_1) = \bar{\alpha}(t_3-t_2) + \bar{\alpha}(t_2-t_1) + 3\left(\frac{\pi}{4} - \frac{\bar{\alpha}_0}{2}\right) - 3i \ln \sqrt{\frac{\pi}{\bar{A}_0}} \tag{4.1.13}$$

Substituting for $\bar{\alpha}$ using the last of (4.1.9) the terms in \bar{B} cancel (the functions \bar{B} and B being the same and the constants \bar{A} and A being the same) and (4.1.13) reduces to

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$$\bar{D}\left(\frac{V}{\hbar}(t_3 - t_1)\right)(t_3 - t_1) = \bar{D}\left(\frac{V}{\hbar}(t_2 - t_1)\right)(t_2 - t_1) + \bar{D}\left(\frac{V}{\hbar}(t_3 - t_2)\right)(t_3 - t_2)$$

giving the functional relation $(x + y)\bar{D}(x + y) = x\bar{D}(x) + y\bar{D}(y)$ which with $y = x$ reduces to $\bar{D}(2x) = \bar{D}(x)$ showing $\bar{D}(x)$ is just a constant \bar{D} .

Hence from (4.1.8) and (4.1.9) using the fact that \bar{B} is the same as B in section 3.1 we arrive at

$$\phi_{x_1 t_1}(x_2 t_2) = \left(\frac{i\pi\hbar}{Am}(t_2 - t_1)\right)^{-1/2} \exp i\left(\bar{A}\frac{m(x_2 - x_1)^2}{\hbar(t_2 - t_1)} + \bar{C}\frac{A_x}{\hbar}(x_2 - x_1) + \left(\bar{D}\frac{A_x^2}{m\hbar} + \frac{1}{3}\gamma\frac{V}{\hbar}\right)(t_2 - t_1)\right) \dots(4.1.14)$$

where γ is the same real constant as in section 3.1 and \bar{A} , \bar{C} and \bar{D} are constants (possibly complex). We now need to establish that result (4.1.14) can satisfy the orthonormal requirement (1.15).

Substituting (4.1.14) (with $t_2 - t_1$ replaced by τ) into (1.15) we get a requirement the same as (1.16) except that A is replaced by \bar{A} , an additional factor

$$e^{\frac{iA_x}{\hbar}(-\bar{C}^*(x_2 - x_1) + \bar{C}(x_2 - x_1'))}$$

appears in the integrand and an additional constant factor

$$e^{\frac{iA_x^2}{m\hbar}(-\bar{D}^* + \bar{D})\tau} \quad (4.1.15)$$

appears on the LHS. (As γ is real the constant term involving γ disappears.) Without the factor (4.1.15) the LHS of (1.16) therefore becomes

$$(\pi)^{-1} \left(\frac{\hbar\tau}{m|\bar{A}|}\right)^{-1} \int_{-\infty}^{\infty} e^{i\frac{m}{\hbar\tau}(-\bar{A}^*(x_2 - x_1)^2 + \bar{A}(x_2 - x_1')^2) + i\frac{A_x}{\hbar}(-\bar{C}^*(x_2 - x_1) + \bar{C}(x_2 - x_1'))} dx_2 \quad (4.1.16)$$

Evaluating the integral in (4.1.16) using the result in Appendix A this equals

$$(\pi)^{-1} \left(\frac{\hbar\tau}{m|\bar{A}|}\right)^{-1} \left(\frac{i\pi}{(\bar{A} - \bar{A}^*)\frac{m}{\hbar\tau}}\right)^{1/2} e^{-i\frac{m}{\hbar\tau}\frac{|\bar{A}|^2}{\bar{A} - \bar{A}^*}(x_1 - x_1')^2 + i\frac{(-\bar{A}^*)(-\bar{C}) + \bar{A}(-\bar{C}^*)}{\bar{A} - \bar{A}^*}\frac{A_x}{\hbar}(x_1 - x_1') - i\frac{1}{4}\frac{(-\bar{C}^* - (-\bar{C}))^2}{\bar{A} - \bar{A}^*}\frac{\hbar\tau}{m}\left(\frac{A_x}{\hbar}\right)^2} \dots(4.1.17)$$

and the integral exists only when

$$\text{Im}(\bar{A} - \bar{A}^*) > 0 \quad (\text{i.e. } \text{Im}(\bar{A}) > 0).$$

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For (4.1.17) times (4.1.15) to equal $\delta(x_1 - x'_1)$ conditions established in Representation 1 of Appendix B must be satisfied. As in section 1 we need to let $\bar{A} - \bar{A}^* \rightarrow 0$, i.e. to make \bar{A} real except for a small positive imaginary part which we let tend to zero. So in the limit \bar{A} is real and equal to α in (3.1.15). But it is also necessary that the factor

$$\frac{(-\bar{A}^*)(-\bar{C}) + \bar{A}(-\bar{C}^*)}{\bar{A} - \bar{A}^*}$$

in (4.1.17) remains finite as $\bar{A} - \bar{A}^* \rightarrow 0$. This requires $-\bar{C} = -\bar{C}^*$ i.e. \bar{C} must be real. The last term in (4.1.17) thus vanishes and (4.1.17) becomes $\delta(x_1 - x'_1)$. So as to not spoil this, the constant factor (4.1.15) must equal 1 i.e. $\bar{D} = \bar{D}^*$ or D must be real.

Replacing the symbol \bar{C} by ε and \bar{D} by β , and forming the product of the transformation functions $\phi_{x_1 t_1}(x_2 t_2)$, $\phi_{y_1 t_1}(y_2 t_2)$ and $\phi_{z_1 t_1}(z_2 t_2)$ we thus arrive at the following form for the transformation function $\phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2)$:

$$\phi_{\mathbf{r}_1 t_1}(\mathbf{r}_2 t_2) = \left(\frac{i\pi\hbar}{\alpha m}(t_2 - t_1)\right)^{-3/2} \exp i\left(\frac{\alpha m(\mathbf{r}_2 - \mathbf{r}_1)^2}{\hbar(t_2 - t_1)} + \frac{\varepsilon}{\hbar} \mathbf{A} \cdot (\mathbf{r}_2 - \mathbf{r}_1) + \left(\beta \frac{A^2}{m\hbar} + \gamma \frac{V}{\hbar}\right)(t_2 - t_1)\right) \dots\dots(4.1.18)$$

where $\alpha, \varepsilon, \beta$ and γ are real numerical constants yet to be found.* The transformation function $\phi_{\mathbf{r}_2 t_2}(\mathbf{r}_1 t_1)$ is of course the conjugate of the RHS of (4.1.18). And for the same reasons as in section 1, the result (4.1.18) holds whether t_2 is greater than or less than t_1 .

It is clear that (4.1.18) satisfies the initial condition (1.5) as required. This follows from Representation 1 of Appendix B (in the case when μ is real).

Assuming $\varepsilon \neq 0$ (and we show in section 5 of Chapter VI that ε must equal 1) it is clear that adding a constant vector (or the gradient of a scalar) to \mathbf{A} alters the probability distribution function. So we cannot claim that such a modification to \mathbf{A} leaves the particle motion unaffected.

4.2 Schrödinger's equation for a particle moving under the action of a general (vector and scalar) potential

The Schrödinger equation for a particle moving in *constant uniform* vector and scalar potentials can be derived in the same way as for a particle in a uniform scalar potential (section 3.2). An equation of the form (2.1) remains valid but now the transformation

* They are later shown to be $\frac{1}{2}, 1, 0$ and -1 respectively. (See section 5 of this Chapter and section 5 of Chapter VI.)

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function in (2.2) is given by (4.1.18) rather than by (3.1.15). So the new kernel $\bar{K}(\mathbf{r} t ; \mathbf{r}_1 t_1)$ is related to the kernel $K(\mathbf{r} t ; \mathbf{r}_1 t_1)$ of section 3.2 by

$$\bar{K}(\mathbf{r} t ; \mathbf{r}_1 t_1) = f(\mathbf{r}, t) K(\mathbf{r} t ; \mathbf{r}_1 t_1) \quad (4.2.1)$$

where

$$f(\mathbf{r}, t) = \exp i \left(\frac{\varepsilon}{\hbar} \mathbf{A} \cdot (\mathbf{r} - \mathbf{r}_1) + \beta \frac{A^2}{m \hbar} (t - t_1) \right) \quad (4.2.2)$$

and we have

$$\nabla \bar{K} = K \nabla f + f \nabla K, \quad \nabla^2 \bar{K} = 2 \nabla K \cdot \nabla f + K \nabla^2 f + f \nabla^2 K.$$

It follows that the new kernel satisfies the differential equation

$$-\frac{\hbar}{i} \frac{\partial \bar{K}}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \bar{K} \cdot \frac{1}{2\alpha} - \gamma V \bar{K} + \frac{i \hbar \varepsilon}{m} \mathbf{A} \cdot \nabla \bar{K} \frac{1}{2\alpha} + \frac{\varepsilon^2 - 4\beta\alpha}{2m} A^2 \bar{K} \frac{1}{2\alpha}. \quad (4.2.3)$$

For on substituting for \bar{K} in (4.2.3) using (4.2.1) and cancelling out terms related by (3.2.1) there remains

$$-\frac{\hbar}{i} \frac{\partial f}{\partial t} K = -\frac{\hbar^2}{2m} \frac{1}{2\alpha} (2 \nabla K \cdot \nabla f + K \nabla^2 f) + \frac{i \hbar \varepsilon}{m} \mathbf{A} \cdot (K \nabla f + f \nabla K) \frac{1}{2\alpha} + \frac{\varepsilon^2 - 4\beta\alpha}{2m} A^2 K f \frac{1}{2\alpha}$$

which is satisfied on account of the fact that (by (4.2.2))

$$\frac{\partial f}{\partial t} = f i \beta \frac{A^2}{m \hbar},$$

$$\nabla f = f i \varepsilon \frac{1}{\hbar} \mathbf{A},$$

$$\nabla^2 f = i \varepsilon \frac{1}{\hbar} \mathbf{A} \cdot \nabla f = -\left(\frac{\varepsilon}{\hbar}\right)^2 f A^2.$$

Under any pure knowledge Y our wave function $\psi(\mathbf{r}, t)$ must clearly satisfy the same differential equation as the new kernel does in (4.2.3). So the Schrödinger equation is now

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi \frac{1}{2\alpha} - \gamma V \psi + \frac{i \hbar \varepsilon}{m} \mathbf{A} \cdot \nabla \psi \frac{1}{2\alpha} + \frac{\varepsilon^2 - 4\beta\alpha}{2m} A^2 \psi \frac{1}{2\alpha}. \quad (4.2.4)$$

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As in section 3, on account of the law of continuous motion and the first law of potential action, this equation must hold not only for constant uniform potentials V and \mathbf{A} but also for potentials $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ varying in any way with position and time.

We will establish the necessary relations $\varepsilon/2\alpha = 1$ and $(\varepsilon^2 - 4\beta\alpha)/2\alpha = -\gamma$ in the next section. The correct values for α and γ (namely $\alpha = 1/2$ and $\gamma = -1$), and therefore for ε (namely $\varepsilon = 1$) and for β (namely $\beta = 0$), are established in section 5 of Chapter VI.

5. Implications of the quantum mechanical principle of equivalence

Consider the motion of a particle of mass m in the general case where any scalar and vector potentials may be present.

Let O and O' be inertial frames, O' moving uniformly relative to O at velocity \mathbf{v} so that at time t it is displaced from O by amount $\mathbf{v}t$. We use the same variable t to denote the time in either inertial frame.

Suppose we have pure knowledge Y of the particle motion relative to O at time $t=0$ (when O and O' momentarily coincide). Taking O to be at rest we will then have a wave function $\psi(\mathbf{r}, t)$ in O satisfying the Schrödinger equation (4.2.4) in which the total vector and scalar potential fields are

$$\left. \begin{aligned} \mathbf{A} &= \mathbf{A}_s + m\mathbf{A}_0 \\ V &= V_s + mV_0 \end{aligned} \right\} \quad (5.1)$$

A_s and V_s being the generally variable potentials due to sources and A_0 and V_0 the supposed constant values of the background fields.

We may if we wish (see section 3.8 of Chapter III) change our mind and claim that O' is at rest and additional background fields $\Delta V_0 = -\frac{1}{2}v^2 - \mathbf{v} \cdot \mathbf{A}_0$ and $\Delta \mathbf{A}_0 = \mathbf{v}$ are present. Then any wave function $\tilde{\psi}'(\mathbf{r}', t)$ in O' satisfies the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \tilde{\psi}'}{\partial t} = -\frac{\hbar^2}{2m} \nabla'^2 \tilde{\psi}' - \frac{1}{2\alpha} \tilde{V} \tilde{\psi}' + \frac{i\hbar\varepsilon}{m} \tilde{\mathbf{A}} \cdot \nabla' \tilde{\psi}' - \frac{1}{2\alpha} + \frac{\varepsilon^2 - 4\beta\alpha}{2m} \tilde{\mathbf{A}}^2 \tilde{\psi}' - \frac{1}{2\alpha} \quad (5.2)$$

in O' where

$$\left. \begin{aligned} \tilde{\mathbf{A}} &= \tilde{\mathbf{A}}_s + m(\mathbf{A}_0 + \mathbf{v}) \\ \tilde{V} &= \tilde{V}_s + m(V_0 - \frac{1}{2}v^2 - \mathbf{v} \cdot \mathbf{A}_0) \end{aligned} \right\} \quad (5.3)$$

\tilde{A}_s and \tilde{V}_s being the potentials of the same sources which however now move with velocity $-\mathbf{v}$ relative to fixed space. By the second law of potential action (section 3.2 of Chapter III) \tilde{A}_s and \tilde{V}_s are related to A_s and V_s by

$$\left. \begin{aligned} \tilde{A}_S(\mathbf{r}', t) &= A_S(\mathbf{r}, t) \\ \tilde{V}_S(\mathbf{r}', t) &= V_S(\mathbf{r}, t) + (-\mathbf{v}) \cdot \mathbf{A}_S(\mathbf{r}, t) \end{aligned} \right\}$$

when $\mathbf{r} = \mathbf{r}' + \mathbf{v}t$. * That is, at any ‘event’ in (classical) space-time

$$\left. \begin{aligned} \tilde{A}_S &= A_S, \\ \tilde{V}_S &= V_S - \mathbf{v} \cdot \mathbf{A}_S \end{aligned} \right\} \quad (5.4)$$

In terms of A_S and V_S (5.4) and (5.3) give for the total potentials at any ‘event’:

$$\left. \begin{aligned} \tilde{A} &= A_S + m(\mathbf{A}_0 + \mathbf{v}) \\ \tilde{V} &= V_S - \mathbf{v} \cdot \mathbf{A}_S + m(V_0 - \frac{1}{2}v^2 - \mathbf{v} \cdot \mathbf{A}_0) \end{aligned} \right\} \quad (5.5)$$

In terms of \mathbf{A} and V in (5.1), equations (5.5) give at any event

$$\left. \begin{aligned} \tilde{A} &= \mathbf{A} + m\mathbf{v} \\ \tilde{V} &= V - \mathbf{v} \cdot \mathbf{A}_S + m(-\frac{1}{2}v^2 - \mathbf{v} \cdot \mathbf{A}_0) = V - \mathbf{v} \cdot \mathbf{A} - \frac{1}{2}mv^2 \end{aligned} \right\} \quad (5.6)$$

the last step following from the first of (5.1).

But we have claimed (see section 3.8 of Chapter III) that our above change in mind concerning the true rest frame and background field values does not affect the possible particle motions relative to any coordinate system. Therefore given our knowledge Y of the particle motion relative to O , the problem of finding the probability distribution $\psi(\mathbf{r}, t)$ in O given O is at rest is *similar* to the problem of finding the probability distribution $\tilde{\psi}(\mathbf{r}, t)$ in O given O' is at rest and the additional background fields are present. This is because for every possible particle motion in the one case there is exactly the same possible motion in the other, and our knowledge Y of the particle motion relative to O is the same in the two cases. Because only our general knowledge is different in the two cases, the similarity principle (5.1.6) of Chapter I applies giving

$$\tilde{\psi}(\mathbf{r}, t) = \psi(\mathbf{r}, t) \quad (5.7)$$

for all \mathbf{r} and t .

Let $\tilde{\psi}'(\mathbf{r}', t)$ be our probability distribution in O' under knowledge Y and supposed knowledge that O' is at rest. Then since propositions claiming the same physical event are fully equivalent we have by the second uniqueness principle (of section 5, Chapter I) that $\tilde{\psi}'(\mathbf{r}', t) = \tilde{\psi}(\mathbf{r}, t)$ when $\mathbf{r} = \mathbf{r}' + \mathbf{v}t$. Therefore by (5.7)

* Here \mathbf{r} denotes the position vector from the origin of O and \mathbf{r}' the position from the origin of O' .

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$$\tilde{\psi}'(\mathbf{r}', t) = \psi(\mathbf{r}, t) \quad (5.8)$$

when $\mathbf{r} = \mathbf{r}' + \mathbf{v}t$, or, more briefly $\tilde{\psi}' = \psi$ at any one and the same 'event'. From (5.8) we thus have at any 'event'

$$\left. \begin{aligned} \tilde{\psi}' &= \psi \\ \frac{\partial \tilde{\psi}'}{\partial t} &= \left(\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi \right) \\ \nabla' \tilde{\psi}' &= \nabla \psi \\ \nabla'^2 \tilde{\psi}' &= \nabla^2 \psi \end{aligned} \right\} \quad (5.9)$$

Now we naturally assume that any knowledge Y of the particle motion relative to O (which is pure knowledge when O is at rest) also qualifies as pure knowledge when O' is taken to be at rest instead. Hence $\tilde{\psi}'$ must satisfy the Schrödinger equation (5.2) in O' , and we obtain by substitution of (5.6) and (5.9) into (5.2) the following equation for $\psi(\mathbf{r}, t)$:

$$\begin{aligned} -\frac{\hbar}{i} \left(\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi \right) &= -\frac{\hbar^2}{2m} \nabla^2 \psi \frac{1}{2\alpha} - \gamma (V - \mathbf{v} \cdot \mathbf{A} - \frac{1}{2} m v^2) \psi + \frac{i\hbar \epsilon}{m} (\mathbf{A} + m\mathbf{v}) \cdot \nabla \psi \frac{1}{2\alpha} \\ &\quad + \frac{\epsilon^2 - 4\beta\alpha}{2m} (A^2 + m^2 v^2 + 2m\mathbf{v} \cdot \mathbf{A}) \psi \frac{1}{2\alpha} \end{aligned}$$

which on account of the fact that $\psi(\mathbf{r}, t)$ must satisfy the Schrödinger equation (4.2.4) in O reduces to

$$-\frac{\hbar}{i} (\mathbf{v} \cdot \nabla \psi) \left(1 - \frac{\epsilon}{2\alpha} \right) = \frac{1}{2} \left(\gamma + \frac{\epsilon^2 - 4\beta\alpha}{2\alpha} \right) m v^2 \psi + \left(\gamma + \frac{\epsilon^2 - 4\beta\alpha}{2\alpha} \right) (\mathbf{v} \cdot \mathbf{A}) \psi. \quad (5.10)$$

Now this must hold for all \mathbf{v} . Equating the coefficients of the second power of \mathbf{v} on both sides gives

$$\gamma + \frac{\epsilon^2 - 4\beta\alpha}{2\alpha} = 0$$

and then the RHS of (5.10) vanishes implying $1 - \frac{\epsilon}{2\alpha} = 0$. Hence the relations

$$\frac{\epsilon}{2\alpha} = 1, \quad \frac{\epsilon^2 - 4\beta\alpha}{2\alpha} = -\gamma. \quad (5.11)$$

CHAPTER V

DERIVATION OF THE MANY PARTICLE SCHRÖDINGER EQUATION

1. The case of constant particle scalar potentials

Consider a system of N distinguishable particles over a certain time period each particle moving under the action of its own constant and uniform external scalar potential without particle/particle interaction. Let $\mathbf{r}_1, \dots, \mathbf{r}_N$ be the positions of particles 1, ... N relative to a fixed coordinate system. Our knowledge regarding the orbital motion of the particles *can* be separate knowledge concerning the motion of each particle on its own, but when the particles have interacted in the past our knowledge is generally inseparable. When inseparable, propositions about the orbital motions of each particle are not logically independent. But the propositions claiming the point $(\mathbf{r}_1, \dots, \mathbf{r}_N)$ in configuration space occupies one or other of equal cubical volume elements $dV (= d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N)$ filling configuration space form a basis in the sample space S of all propositions concerning the positions and momenta of all N particles over a specified time period. Using this basis and under *pure* knowledge Y of the motion of the system we will have a time dependent wave function $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ where

$$\Phi(d^3\mathbf{r}_1, \dots, d^3\mathbf{r}_N, t | Y) = \psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t) \sqrt{d^3\mathbf{r}_1} \dots \sqrt{d^3\mathbf{r}_N} \quad (1.1)$$

Sample space S is the combination $S_{r_1} \dots S_{r_N}$ of sample spaces S_{r_1}, \dots, S_{r_N} (of the kind described in section 2.2 of Chapter III) for each particle, and since we are presently assuming no particle/particle interaction, the sample spaces S_{r_1}, \dots, S_{r_N} and S itself are all closed. Referring to the position of the point P in configuration space, position/position transformation functions between times t' and t are therefore the products of the position/position transformation functions for the separate particles (see section 5 of Chapter II) and the relationship between the wave function at time t and the wave function at time t' is, by Feynman's law,

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t) = \int \dots \int \phi_{r'_1 \dots r'_N, t'}(\mathbf{r}_1, \dots, \mathbf{r}_N, t) \psi(\mathbf{r}'_1, \dots, \mathbf{r}'_N, t') d^3\mathbf{r}'_1 \dots d^3\mathbf{r}'_N \quad (1.2)$$

where

$$\phi_{r'_1 \dots r'_N, t'}(\mathbf{r}_1, \dots, \mathbf{r}_N, t) = \phi_{r'_1}(\mathbf{r}_1, t) \dots \phi_{r'_N}(\mathbf{r}_N, t) \quad (1.3)$$

each factor on the RHS of (1.3) being the transformation function for a single particle in its constant potential field (given by (3.1.15) of Chapter IV).

As noted in section 3.2 of Chapter IV the transformation function $\phi_i = \phi_{\mathbf{r}_i t}$ or kernel K_i for the i^{th} particle satisfies the Schrödinger equation (3.2.1) of Chapter IV. Thus

$$-\frac{\hbar}{i} \frac{\partial \phi_i}{\partial t} = -\frac{\hbar^2}{2m_i} \nabla_i^2 \phi_i \cdot \frac{1}{2\alpha} - \gamma V_i \phi_i. \quad (1.4)$$

where m_i is the mass of the i^{th} particle, V_i the constant potential of the i^{th} particle and ∇_i^2 the Laplacian operator in the i^{th} particle space coordinates. The transformation function $\psi = \phi_{\mathbf{r}'_1, \dots, \mathbf{r}'_N, t'}(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ for given $\mathbf{r}'_1, \dots, \mathbf{r}'_N, t'$ therefore satisfies the N -particle Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 \psi \frac{1}{2\alpha} - \gamma V \psi \quad (1.5)$$

where

$$V = \sum_{i=1}^N V_i \quad (1.6)$$

is the constant system potential. This result follows by direct substitution of (1.3) into (1.5) and use of (1.4).

Being a linear combination of the $\phi_{\mathbf{r}'_1, \dots, \mathbf{r}'_N, t'}(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ for different $\mathbf{r}'_1, \dots, \mathbf{r}'_N, t'$, as in (1.2), any wave function $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ (in the case of constant potentials) must also satisfy the Schrödinger equation (1.5).

2. Case of a general system potential

A system of particles may move under the influence of variable external scalar potentials *and* inter-particle potentials. The system potential is then a function $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$. In particular it may (as is common) take the form

$$V(\mathbf{r}_1, \dots, \mathbf{r}_N, t) = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_{i=1}^N V_i(\mathbf{r}_i) \quad (2.1)$$

where $V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|)$ (equal to $V_{ji}(|\mathbf{r}_j - \mathbf{r}_i|)$) is the potential energy between particles i and j , i.e. a known function of the distance between the particles (possibly a different function and different kind of potential for each pair of particles). By convention

$$V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) = 0, \quad \text{for } i = j \quad (2.2)$$

and $V_i(\mathbf{r}_i)$ is the known potential energy of the i^{th} particle in the external field. The $V_i(\mathbf{r}_i)$ and the $V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|)$ may be functions of the time t also.

The proof that (1.5) holds for *any* known system potential $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ (of the form (2.1) or of more general form) is conducted in a manner similar to the one used in section 3.2 of Chapter IV in the case of a single particle.

Consider first the case of each particle moving in its own *constant* potential field. The change in ψ in a short time is given by (1.5) and depends, at any point of configuration space, only on the local values of $\nabla_i^2 \psi$, ψ and V in that space. By (1.5), after a short time dt the value of $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ changes thus:

$$\psi \rightarrow \psi + \frac{i}{\hbar} \left(\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 \psi \frac{1}{2\alpha} + \gamma V \psi \right) dt. \quad (2.3)$$

Now consider the case of any system potential $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$. Suppose we know $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ everywhere at time t and set ourselves the problem of calculating $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t + dt)$ inside a small volume element dV of configuration space any short time dt later. For this purpose we consider the sample space S' of propositions regarding the motion of the representative point in configuration space from time t onwards. Let dV' be a small volume element of configuration space enclosing dV .

We know that the motion of the representation point during time t to $t + dt$, should it be in dV then, is affected by the value of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ in dV' at that time (but not by its local spatial or temporal derivatives at that time) nor by the system potential outside dV' between times t and $t + dt$, nor by future values of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ anywhere. Values of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ somewhere at *earlier* times might affect the motion of the representative point during time t to $t + dt$. But since we have pure knowledge in S' (expressed by $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ at time t), knowledge of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ at earlier times is redundant.

We know that the particles do not move infinitely fast so that our knowledge regarding the position of the representation point at time t outside the small volume element dV' enclosing dV is superfluous for our present purpose. Therefore our problem is *similar* to the one in which the potential is constant from time t to time $t + dt$ and uniform throughout configuration space and equal to the local value of $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ at the position of dV and at the time t in question. But this means that (2.3) must hold also for the change in $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ over any short enough time even when $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ is non-uniform, time dependent and of any form. More precisely the similarity principle implies that for $\mathbf{r}_1, \dots, \mathbf{r}_N$ in dV and after any short time interval dt

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t + dt) = \left(\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t) + \frac{i}{\hbar} \left(\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 \psi \frac{1}{2\alpha} + \gamma V(\mathbf{r}_1, \dots, \mathbf{r}_N, t) \psi \right) dt \right) e^{i\beta}$$

where β is a real constant independent of dt . But for $dt \rightarrow 0$ we must have $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t + dt) \rightarrow \psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ so that β can only be zero and $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ must satisfy

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 \psi \frac{1}{2\alpha} - \gamma V(\mathbf{r}_1, \dots, \mathbf{r}_N, t) \psi \quad (2.4)$$

in any short enough time interval.

Being valid for any short enough time interval and for any volume element dV of configuration space, (2.4) is valid for all times and positions in configuration space and this establishes the Schrödinger equation for a many particle system with a general system potential.

3. Inclusion of vector potentials

In non-relativistic quantum mechanics there are no inter-particle *vector* potentials, so we have only to include *external* vector potentials $\mathbf{A}_i(\mathbf{r}_i, t)$ for each particle with $\nabla_i \cdot \mathbf{A}_i = 0$ for each i .

The derivation of the many particle Schrödinger equation for a general system potential $V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ and general external vector potentials may be conducted in the same way as in the case of a general system potential. The derivation goes as follows.

In the case each particle moves under the action of its own (external) *constant uniform* scalar and vector potential fields the transformation function $\phi_i = \phi_{\mathbf{r}_i'}(\mathbf{r}_i, t)$ for the i^{th} particle (given by (4.1.18) of Chapter IV) satisfies the individual Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \phi_i}{\partial t} = -\frac{\hbar^2}{2m_i} \nabla_i^2 \phi_i \frac{1}{2\alpha} - \gamma V_i \phi_i + \frac{i\hbar \epsilon}{m_i} \mathbf{A}_i \cdot \nabla_i \phi_i \frac{1}{2\alpha} + \frac{\epsilon^2 - 4\beta\alpha}{2m_i} A_i^2 \phi_i \frac{1}{2\alpha}. \quad (3.1)$$

given by (4.2.4) of Chapter IV with the V_i and \mathbf{A}_i constants. The transformation function $\psi = \phi_{\mathbf{r}'_1, \dots, \mathbf{r}'_N, t'}(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ for given $\mathbf{r}'_1, \dots, \mathbf{r}'_N, t'$ therefore satisfies the N -particle Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 \psi \frac{1}{2\alpha} - \gamma V \psi + \sum_{i=1}^N \left(\frac{i\hbar \epsilon}{m_i} \mathbf{A}_i \cdot \nabla_i \psi \frac{1}{2\alpha} + \frac{\epsilon^2 - 4\beta\alpha}{2m_i} A_i^2 \psi \frac{1}{2\alpha} \right) \quad (3.2)$$

as can be confirmed by substitution of (1.3) and (1.6) into (3.2) and use of (3.1). As any wave function $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ can be expressed in the form (1.2) it too must satisfy (3.2).

V. *The many particle Schrödinger equation*

In the case of a general system potential $V = V(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ and general (space and time dependent) external vector potentials $\mathbf{A}_i(\mathbf{r}_i, t)$ for each particle, (3.2) must still hold for the wave function $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ representing any pure state of knowledge of the system's motion. This follows (as in section 2) from the redundancy (under pure knowledge) of the knowledge of earlier potentials, the law of continuous motion, the first law of potential action and the similarity principle.

CHAPTER VI
MOMENTUM

1. Properties of momentum

In relation to the orbital motion of a single particle, whether it moves freely or under the action of potentials, there is, axiomatically, at any one time, an internal property called ‘momentum’ (a vector \mathbf{p} with units MLT^{-1}) relative to each stationary coordinate system. The momentum is not changed if the coordinate system occupies the same orientation the other way (see section 3.9 of Chapter III). And, as in classical mechanics, at any time t and under any rotation of the coordinate system about an axis through the origin, the Cartesian components of \mathbf{p} transform like the Cartesian components of an ordinary vector. But (unlike the situation in classical mechanics), at any one time t , the momenta $\mathbf{p}, \mathbf{p}', \dots$ of a particle relative to stationary coordinate systems O, O', \dots whose origins occupy different points in fixed space, are *distinct* physical properties.*

In the closed sample space S_r (of section 2.2 Chapter III) for orbital motion of a single particle, the momentum relative to any one fixed coordinate system is a *basic* property. In the case of a free particle, or of a particle moving under the action of a *uniform* scalar and/or *uniform* vector potential, the Cartesian components of momentum in three mutually perpendicular directions x, y and z are basic properties in the separately closed sample spaces S_x, S_y and S_z (of section 2.2 Chapter III).

We now introduce the following law applying at any one time:

The law of constancy of momentum under coordinate displacement

Let O and O' be any pair of fixed coordinate systems, the second being displaced a distance Δ relative to the first, then the momentum \mathbf{p} relative to O and the momentum \mathbf{p}' relative to O' are always equal. But (with $\mathbf{p} = \mathbf{p}'$) the propositions ‘ \mathbf{p} in O ’ and ‘ \mathbf{p}' in O' ’ (claiming the values \mathbf{p} and \mathbf{p}' apply in O and O' respectively) imply one another with phases of implication that are equal to zero only when $\mathbf{p} \cdot \Delta = 2\pi n \hbar$ where n is an integer.

Now let free orbital motion of a single particle be considered relative to one or other of two fixed Cartesian coordinate systems O and O' the second being displaced a distance Δ relative to the first. Then, as we have said, the particle has, at any one time, a momentum \mathbf{p} relative to O and another (equal) momentum \mathbf{p}' relative to O' and either

* The momenta $\mathbf{p}, \mathbf{p}', \dots$ relative to O, O', \dots must therefore be somehow encoded in the internal motion associated with momentum, much as the z components of spin in coordinate systems of different orientation are encoded in the internal motion associated with spin.

property may serve as a basis, as may the position \mathbf{r} of the particle relative to coordinates O at the same time. We will seek the transformation functions between \mathbf{p} and \mathbf{p}' (the ‘momentum/momentum transformation functions’) and the transformation functions between \mathbf{p} and \mathbf{r} (the ‘momentum/position transformation functions’). The problems of finding these transformation functions for different kinds of particle are taken to be equivalent.

2. Derivation of the momentum/momentum transformation functions for a free particle

Dividing momentum space up into equal infinitesimal cubical parts, we seek the transformation function $\Phi(d^3\mathbf{p}'|d^3\mathbf{p})$ and its conjugate $\Phi(d^3\mathbf{p}|d^3\mathbf{p}')$. In either of these, ‘ $d^3\mathbf{p}$ ’ is the proposition claiming that ‘relative to O , \mathbf{p} lies in element $d^3\mathbf{p}$ at time t ’, and ‘ $d^3\mathbf{p}'$ ’ is the proposition claiming ‘relative to O' , \mathbf{p}' lies in element $d^3\mathbf{p}'$ at time t ’ O' being displaced by \mathcal{A}' relative to O .

The distribution $\Phi(d^3\mathbf{p}'|d^3\mathbf{p})$ must be proportional to $\sqrt{d^3\mathbf{p}}$ in order that in the normalisation requirement

$$\sum_{d^3\mathbf{p}} |\Phi(d^3\mathbf{p}'|d^3\mathbf{p})|^2 = 1 \quad (2.1)$$

the LHS becomes an ordinary integral. Similarly the inverse transformation function $\Phi(d^3\mathbf{p}|d^3\mathbf{p}')$, the conjugate of $\Phi(d^3\mathbf{p}'|d^3\mathbf{p})$, must be proportional to $\sqrt{d^3\mathbf{p}'}$. So $\Phi(d^3\mathbf{p}'|d^3\mathbf{p})$ and $\Phi(d^3\mathbf{p}|d^3\mathbf{p}')$ have the forms*

$$\left. \begin{aligned} \Phi(d^3\mathbf{p}'|d^3\mathbf{p}) &= \phi_{p'}(\mathbf{p}) \sqrt{d^3\mathbf{p}'} \sqrt{d^3\mathbf{p}} \\ \Phi(d^3\mathbf{p}|d^3\mathbf{p}') &= \phi_p(\mathbf{p}') \sqrt{d^3\mathbf{p}} \sqrt{d^3\mathbf{p}'} \end{aligned} \right\} \quad (2.2)$$

and we seek the functions $\phi_{p'}(\mathbf{p})$ and $\phi_p(\mathbf{p}')$ where

$$\phi_p(\mathbf{p}') = (\phi_{p'}(\mathbf{p}))^* . \quad (2.3)$$

Of course, when $\mathcal{A}' = 0$, the first and second laws of extreme values (section 2.2.2 of Chapter I) and the fact that any proposition implies itself with zero phase of implication make

* We use, for brevity, the same symbol ϕ to denote different functions $\phi_{p'}(\mathbf{p})$ and $\phi_p(\mathbf{p}')$.

$$\Phi(d^3\mathbf{p}|d^3\mathbf{p}') = \delta_{d^3\mathbf{p},d^3\mathbf{p}'} = \begin{cases} 1 & d^3\mathbf{p} = d^3\mathbf{p}' \\ 0 & d^3\mathbf{p} \neq d^3\mathbf{p}' \end{cases}.$$

This means that in (2.2)

$$\phi_{p'}(\mathbf{p})\Big|_{\mathcal{A}' \rightarrow 0} = \delta(\mathbf{p} - \mathbf{p}'), \quad (2.4)$$

where the delta function is

$$\delta(\mathbf{p} - \mathbf{p}') = (1/d^3\mathbf{p}')\delta_{d^3\mathbf{p},d^3\mathbf{p}'}.$$

The functions $\phi_{p'}(\mathbf{p})$ (and therefore the functions $\phi_p(\mathbf{p}')$) are universal functions of \mathbf{p} , \mathbf{p}' and \mathcal{A}' i.e. they are functions independent of the position of the origin of the coordinates \mathbf{O} and independent of the time to which \mathbf{p}' (and \mathbf{p}) refer. This is because the problem of finding the distributions $\phi_{p'}(\mathbf{p})$ relating to fixed coordinates \mathbf{O} and \mathbf{O}' at a time t for any number of different displacements \mathcal{A}' of \mathbf{O}' from \mathbf{O} , i.e. the problem of finding the probabilities $\phi_{p'\mathcal{A}'}(\mathbf{p})$ where \mathcal{A}' is made explicit, is (because of the homogeneity of time and space) *similar* to the problem of finding the distributions $\tilde{\phi}_{p'\mathcal{A}'}(\mathbf{p})$ relating to any other pair of fixed coordinates $\tilde{\mathbf{O}}$ and $\tilde{\mathbf{O}'}$ at any other time \tilde{t} for the same displacements \mathcal{A}' of $\tilde{\mathbf{O}'}$ from $\tilde{\mathbf{O}}$. Hence

$$\tilde{\phi}_{p'\mathcal{A}'}(\mathbf{p}) = \phi_{p'\mathcal{A}'}(\mathbf{p})e^{i\beta} \quad (2.5)$$

where β is a real constant, i.e. independent of \mathbf{p} , \mathbf{p}' and \mathcal{A}' , but possibly a function of \tilde{t} and of the position of the origin $\tilde{\mathbf{O}}$.^{*} But for $\mathcal{A}' \rightarrow 0$, $\tilde{\phi}_{p'\mathcal{A}'}(\mathbf{p})$ and $\phi_{p'\mathcal{A}'}(\mathbf{p})$ are certainly equal (both equal to $\delta(\mathbf{p} - \mathbf{p}')$ by (2.4)) so in (2.5), β can only be zero.

To find $\phi_p(\mathbf{p})$ (where we now drop the \mathcal{A}' for simplicity) we first note that the law of constancy of momentum under coordinate displacement in section 1 gives, by the first law of extreme values (section 2.2.2 Chapter I), the necessary form

$$\phi_p(\mathbf{p}) = \delta(\mathbf{p} - \mathbf{p}')e^{i\alpha(\mathbf{p},\mathcal{A}')} \quad (2.6)$$

where $\alpha(\mathbf{p},\mathcal{A}')$ is an, as yet, a generally unknown phase – a real differentiable function of \mathbf{p} and \mathcal{A}' satisfying

^{*} (2.5) follows from (5.1.2) of Chapter I in the case of common general knowledge (i.e. with $G_j^{(1)} = G_j^{(2)} = G_j$) i labelling propositions \mathbf{p} (or $d^3\mathbf{p}$) and j labelling propositions $\mathbf{p}'\mathcal{A}'$ (or $d^3\mathbf{p}'\mathcal{A}'$).

$$\alpha(\mathbf{p}, \mathbf{A}') = 0 \quad \text{only when} \quad \mathbf{p} \cdot \mathbf{A}' = 2\pi n \hbar. \quad (2.7)$$

To help calculate $\alpha(\mathbf{p}, \mathbf{A}')$ consider a third fixed coordinate system O'' displaced a distance \mathbf{A}'' relative to O . Feynman's law

$$\Phi(d^3\mathbf{p} | d^3\mathbf{p}'') = \sum_{d^3\mathbf{p}'} \Phi(d^3\mathbf{p} | d^3\mathbf{p}') \Phi(d^3\mathbf{p}' | d^3\mathbf{p}'')$$

gives the necessary relation

$$\phi_{p''}(\mathbf{p}) = \int \phi_{p'}(\mathbf{p}) \phi_{p'}(\mathbf{p}') d^3\mathbf{p}' \quad (2.8)$$

between the representations $\phi_{p''}(\mathbf{p})$ and $\phi_{p'}(\mathbf{p}')$ of the same pure state of knowledge (that momentum relative to O'' has value \mathbf{p}''). Substituting (2.6) in (2.8) gives

$$\delta(\mathbf{p} - \mathbf{p}'') e^{i\alpha(\mathbf{p}, \mathbf{A}'')} = \int \delta(\mathbf{p} - \mathbf{p}') e^{i\alpha(\mathbf{p}, \mathbf{A}')} \cdot \delta(\mathbf{p}' - \mathbf{p}'') e^{i\alpha(\mathbf{p}', \mathbf{A}' - \mathbf{A}')} d^3\mathbf{p}'$$

and hence

$$\alpha(\mathbf{p}, \mathbf{A}'') = \alpha(\mathbf{p}, \mathbf{A}') + \alpha(\mathbf{p}, \mathbf{A}'' - \mathbf{A}').$$

So $\alpha(\mathbf{p}, \mathbf{A})$ (we now drop the prime on the delta) must be a homogeneous linear function of \mathbf{A} , i.e. $\alpha(\mathbf{p}, \mathbf{A}) = \mathbf{f}(\mathbf{p}) \cdot \mathbf{A}$ and hence

$$\phi_{p'}(\mathbf{p}) = \delta(\mathbf{p} - \mathbf{p}') e^{i\mathbf{f}(\mathbf{p}) \cdot \mathbf{A}}. \quad (2.9)$$

Now taking the Cartesian coordinate systems O and O' to have the same orientation we could conduct a similar argument for each of the components of momentum and hence come up with the forms

$$\left. \begin{aligned} \phi_{p'_x}(p_x) &= \delta(p_x - p'_x) e^{ig(p_x) \Delta_x} \\ \phi_{p'_y}(p_y) &= \delta(p_y - p'_y) e^{ig(p_y) \Delta_y} \\ \phi_{p'_z}(p_z) &= \delta(p_z - p'_z) e^{ig(p_z) \Delta_z} \end{aligned} \right\} \quad (2.10)$$

where, by the isotropy of space and the similarity principle, g must be the same real valued function in each case.

Since the phases in (2.10) must be dimensionless and since we have at our disposal only one fundamental physical constant, i.e. \hbar^* , we only get non-dimensional

* or \hbar and the particle mass if this should be considered relevant

phases by making g a linear homogeneous function of its argument, i.e. $g(p_x) = -\beta p_x/\hbar$ where β is a real numerical constant.

Now $\phi_{p'}(\mathbf{p})$ is the product of the distributions (2.10) and so we arrive at the result

$$\phi_{p'}(\mathbf{p}) = \delta(\mathbf{p} - \mathbf{p}') e^{-i\beta \mathbf{p} \cdot \mathbf{A}/\hbar} \quad (2.11)$$

where β is a universal real numerical constant independent of particle type. It follows from (2.7) that β can only be ± 1 . It cannot be $\pm m$ where m is an integer greater than 1 for then $\alpha(\mathbf{p}, \mathbf{A})$, equal to $-\beta \mathbf{p} \cdot \mathbf{A}/\hbar$ in (2.11), is for certain zero (modulo 2π) for a value of $\mathbf{p} \cdot \mathbf{A}$ not equal to $2\pi n\hbar$ (i.e. for $\mathbf{p} \cdot \mathbf{A} = 2\pi n\hbar/m$).

The choice of the value $+1$ or -1 for β is arbitrary (see section 8 of Chapter I). By convention it is taken as $+1$ and so we finally arrive at the transformation functions

$$\left. \begin{aligned} \phi_{p'}(\mathbf{p}) &= \delta(\mathbf{p} - \mathbf{p}') e^{-i\mathbf{p} \cdot \mathbf{A}/\hbar} \\ \phi_p(\mathbf{p}') &= \delta(\mathbf{p} - \mathbf{p}') e^{i\mathbf{p} \cdot \mathbf{A}/\hbar} \end{aligned} \right\} \quad (2.12)$$

3. Derivation of the momentum/position transformation functions for a free particle

Dividing space up into equal infinitesimal elements $d^3\mathbf{r}$ labelled by the variable \mathbf{r} , we now derive the form of the transformation functions $\Phi(d^3\mathbf{r}|d^3\mathbf{p})$ and $\Phi(d^3\mathbf{p}|d^3\mathbf{r})$ in any fixed Cartesian coordinate system O , the propositions ' $d^3\mathbf{r}$ ' and ' $d^3\mathbf{p}$ ' referring to one and the same time t .

In the same way as we derived the forms (2.2) we see at once that

$$\Phi(d^3\mathbf{r}|d^3\mathbf{p}) = \phi_p(\mathbf{r}) \sqrt{d^3\mathbf{p}} \sqrt{d^3\mathbf{r}}, \quad \Phi(d^3\mathbf{p}|d^3\mathbf{r}) = \phi_r(\mathbf{p}) \sqrt{d^3\mathbf{r}} \sqrt{d^3\mathbf{p}} \quad (3.1)$$

where

$$\phi_r(\mathbf{p}) = (\phi_p(\mathbf{r}))^* \quad (3.2)$$

and both functions $\phi_p(\mathbf{r})$ and $\phi_r(\mathbf{p})$ must have the same units as $\hbar^{-3/2}$.

We assume the same physical properties of momentum as we did in section 1 and find $\phi_p(\mathbf{r})$ using the results of section 2 and Feynman's law.

First we show $\phi_p(\mathbf{r})$ is a universal function of \mathbf{r} and \mathbf{p} , i.e. the same in all fixed coordinate systems and at all times.

Under a shift δ of coordinates we obtain new fixed coordinates O' . By the homogeneity of space, $\phi'_p(\mathbf{r})$ in the new system must (by *similarity*) be the same *function* to within a constant phase factor. We write this as

$$\phi'_p(\mathbf{r}) = \phi_p(\mathbf{r})e^{i\beta}$$

the prime referring to O' . Here β is independent of \mathbf{r} and \mathbf{p} but might depend on δ . With \mathbf{p} equal to zero this gives

$$\phi'_0(\mathbf{r}) = \phi_0(\mathbf{r})e^{i\beta(\delta)} \quad (3.3)$$

By the law of constancy of momentum under coordinate displacement, ' $\mathbf{p} = 0$ in O ' \Leftrightarrow ' $\mathbf{p}' = 0$ in O' '. Also if \mathbf{r}' in O' represents the same point as \mathbf{r} represents in O then $\mathbf{r}' \Leftrightarrow \mathbf{r}$. So by the second uniqueness principle (section 5 of Chapter I)

$$\phi'_0(\mathbf{r}') = \phi_0(\mathbf{r}),$$

when $\mathbf{r} = \mathbf{r}' + \delta$. This gives, by (3.3) with \mathbf{r} replaced by \mathbf{r}' ,

$$\phi_0(\mathbf{r}) = \phi_0(\mathbf{r}')e^{i\beta(\delta)}$$

when $\mathbf{r} = \mathbf{r}' + \delta$. But when we know just that $\mathbf{p} = 0$, there is no way our probability density $\phi_0(\mathbf{r})$ can vary from point to point in space. Because of the homogeneity of space and the lack of any special distance or direction in space* we are indifferent with regard to claiming particle location in one or other of the (equal) elements $d^3\mathbf{r}$. Neither can we distinguish different elements $d^3\mathbf{r}$ in an *absolute* manner. By the principle of indifference (5.2.2) of Chapter I this means $\phi_0(\mathbf{r})$ can only be a (generally complex) constant, i.e.

$$\phi_0(\mathbf{r}) = \phi_0(\mathbf{r}') = \text{const.}, \quad (3.4)$$

and therefore $\beta(\delta)$ can only be zero. Hence $\phi_p(\mathbf{r})$ is the same function in any fixed coordinate system however positioned.

Let $\phi'_p(\mathbf{r})$ now stand for the transformation functions in the same coordinate system O but at a time τ later on. Then the homogeneity of time and the similarity principle gives

* It is obvious that there is no special direction in space. And there can be no special distance either since no quantity of dimension of length can be formed from \hbar alone or from \hbar and the particle mass if this mass should be considered relevant.

$$\phi'_p(\mathbf{r}) = \phi_p(\mathbf{r})e^{i\beta(\tau)}$$

where $\beta(\tau)$ is independent of \mathbf{r} and \mathbf{p} but might depend on τ with $\beta(0) = 0$. But since there is no dimensionless combination of τ and \hbar^* , $\beta(\tau)$ can only be a numerical constant independent of τ and because $\beta(0) = 0$ it can only be zero.

Hence $\phi_p(\mathbf{r})$ is the same function at any time as well as being the same function in any fixed coordinate system.

Next we use Feynman's law in the form

$$\Phi(d^3\mathbf{r}|d^3\mathbf{p}) = \sum_{d^3\mathbf{r}', d^3\mathbf{p}'} \Phi(d^3\mathbf{r}|d^3\mathbf{r}')\Phi(d^3\mathbf{r}'|d^3\mathbf{p}')\Phi(d^3\mathbf{p}'|d^3\mathbf{p}) \quad (3.5)$$

where the prime refers to a fixed coordinate system O' displaced from O by distance \mathbf{A} . In O' we have

$$\Phi(d^3\mathbf{r}'|d^3\mathbf{p}') = \phi_{p'}(\mathbf{r}')\sqrt{d^3\mathbf{p}'}\sqrt{d^3\mathbf{r}'}$$

and since propositions ' \mathbf{r}' in O' ' and ' $\mathbf{r} = \mathbf{r}' + \mathbf{A}$ in O ' imply one another with zero phases of implication

$$\Phi(d^3\mathbf{r}|d^3\mathbf{r}') = \delta(\mathbf{r} - (\mathbf{r}' + \mathbf{A}))\sqrt{d^3\mathbf{r}'}\sqrt{d^3\mathbf{r}}$$

and from (2.2) we have

$$\Phi(d^3\mathbf{p}'|d^3\mathbf{p}) = \phi_p(\mathbf{p}')\sqrt{d^3\mathbf{p}}\sqrt{d^3\mathbf{p}'}$$

where by (2.12)

$$\phi_p(\mathbf{p}') = \delta(\mathbf{p} - \mathbf{p}')e^{i\mathbf{p}\cdot\mathbf{A}/\hbar}.$$

Hence (3.5) gives

$$\begin{aligned} \phi_p(\mathbf{r}) &= \iint \delta(\mathbf{r}' - (\mathbf{r} - \mathbf{A}))\phi_{p'}(\mathbf{r}')\phi_p(\mathbf{p}')d^3\mathbf{r}'d^3\mathbf{p}' = \int \phi_{p'}(\mathbf{r} - \mathbf{A})\delta(\mathbf{p} - \mathbf{p}')e^{i\mathbf{p}\cdot\mathbf{A}/\hbar}d^3\mathbf{p}' \\ &= \phi_p(\mathbf{r} - \mathbf{A})e^{i\mathbf{p}\cdot\mathbf{A}/\hbar} \end{aligned}$$

which must hold for all \mathbf{A} . With \mathbf{A} infinitesimal it gives

* or of τ , \hbar and the particle mass

$$\frac{\partial \phi_p(\mathbf{r})}{\partial \mathbf{r}} \cdot \mathbf{A} = i(\mathbf{p} \cdot \mathbf{A} / \hbar) \phi_p(\mathbf{r})$$

or

$$\frac{\hbar}{i} \frac{\partial \phi_p(\mathbf{r})}{\partial \mathbf{r}} = \mathbf{p} \phi_p(\mathbf{r}).$$

So $\phi_p(\mathbf{r})$ must be an eigenfunction of $\frac{\hbar}{i} \frac{\partial}{\partial \mathbf{r}}$ with eigenvalue \mathbf{p} . Solving this equation gives

$$\phi_p(\mathbf{r}) = k(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{r} / \hbar}$$

where $k(\mathbf{p})$ is a complex function of \mathbf{p} which must be such as to satisfy the orthonormal condition

$$\sum_{d^3 \mathbf{r}} \Phi^*(d^3 \mathbf{r} | d^3 \mathbf{p}) \Phi(d^3 \mathbf{r} | d^3 \mathbf{p}') = \delta_{d^3 \mathbf{p}, d^3 \mathbf{p}'} = d^3 \mathbf{p} \delta(\mathbf{p} - \mathbf{p}')$$

where \mathbf{p}' now stands for another value of \mathbf{p} in the same coordinate system O . This orthonormality condition requires

$$\int \phi_p^*(\mathbf{r}) \phi_{p'}(\mathbf{r}) d^3 \mathbf{r} = k^*(\mathbf{p}) k(\mathbf{p}') \int \exp(i \frac{1}{\hbar} (\mathbf{p}' - \mathbf{p}) \cdot \mathbf{r}) d^3 \mathbf{r} = \delta(\mathbf{p} - \mathbf{p}'). \quad (3.6)$$

Using the result

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(ixt) dt = \delta(x)$$

(see Representation 4 of Appendix B) we have

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(i \frac{x}{\hbar} (p'_x - p_x)) d(\frac{x}{\hbar}) = \delta(p_x - p'_x)$$

and similarly for the y and z components. Forming the product of these and substituting the result into (3.6) shows $|k(\mathbf{p})| = (2\pi\hbar)^{-3/2}$. So we have the following form for $\phi_p(\mathbf{r})$:

$$\phi_p(\mathbf{r}) = (2\pi\hbar)^{-3/2} \exp(i\mathbf{p} \cdot \mathbf{r} / \hbar + i\angle k(\mathbf{p})). \quad (3.7)$$

Now we can conduct a similar argument with each of the Cartesian components of \mathbf{p} and \mathbf{r} and hence come up with the forms

$$\left. \begin{aligned} \phi_{p_x}(x) &= (2\pi\hbar)^{-1/2} \exp(ip_x x/\hbar + if_1(p_x)) \\ \phi_{p_y}(y) &= (2\pi\hbar)^{-1/2} \exp(ip_y y/\hbar + if_2(p_y)) \\ \phi_{p_z}(z) &= (2\pi\hbar)^{-1/2} \exp(ip_z z/\hbar + if_3(p_z)) \end{aligned} \right\} \quad (3.8)$$

where, by the isotropy of space and the similarity principle, the real valued (and necessarily continuous) functions f_1, f_2 and f_3 must, apart from an arbitrary additive constant, be the same in each case. Since we have at our disposal only one fundamental physical constant \hbar and a momentum component in each case*, we only get non-dimensional phases by making f_1, f_2 and f_3 real numerical constants.

Since $\phi_p(\mathbf{r})$ is the product of the distributions (3.8) we arrive at the following forms for $\phi_p(\mathbf{r})$ and $\phi_r(\mathbf{p})$:

$$\left. \begin{aligned} \phi_p(\mathbf{r}) &= (2\pi\hbar)^{-3/2} \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar + i\varepsilon) \\ \phi_r(\mathbf{p}) &= (2\pi\hbar)^{-3/2} \exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar - i\varepsilon) \end{aligned} \right\} \quad (3.9)$$

where $\varepsilon (= f_1 + f_2 + f_3)$ is an indeterminate constant phase independent of \mathbf{p} and \mathbf{r} .[†] By convention we may choose to take $f_1 = f_2 = f_3 = 0$ in (3.8) so long as we make appropriate choices of the indeterminate absolute phases of any other wave functions that are related to (and therefore not independent of) $\phi_{p_x}(x), \phi_{p_y}(y)$ and $\phi_{p_z}(z)$ (see section 3.5 of Chapter I). In particular we must then put $\varepsilon = 0$ in (3.9) giving

$$\left. \begin{aligned} \phi_p(\mathbf{r}) &= (2\pi\hbar)^{-3/2} \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar) \\ \phi_r(\mathbf{p}) &= (2\pi\hbar)^{-3/2} \exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar) \end{aligned} \right\} \quad (3.10)$$

Results (3.9) or (3.10) hold in any fixed coordinate system and at any time, and for any kind of particle moving in free space.

* and the particle mass if this is considered relevant

[†] The first of (3.9) is evidently consistent with the principle of indifference. For knowing only \mathbf{p} we are clearly indifferent with regard to particle position so that $|\phi_p(\mathbf{r})|^2$ should be constant, and it is. Also, when $\mathbf{p} \neq 0$ the existence of a characteristic length $\hbar/|\mathbf{p}|$ and direction $\mathbf{p}/|\mathbf{p}|$ enables us to absolutely distinguish between different position components in the direction $\mathbf{p}/|\mathbf{p}|$ so we are not absolutely indifferent with regard to such position components and accordingly $\angle\phi_p(\mathbf{r})$ should not necessarily be constant in the direction of $\mathbf{p}/|\mathbf{p}|$, and it is not.

4. The transformation functions under motion in an external field

In any fixed coordinate system and in the presence of any finite (generally non-uniform and time dependent) scalar potential field $V(\mathbf{r}, t)$ and/or vector potential field $\mathbf{A}(\mathbf{r}, t)$, the transformation functions $\phi_p(\mathbf{r})$, $\phi_r(\mathbf{p})$, $\phi_p(\mathbf{p})$ and $\phi_p(\mathbf{p}')$ remain the same. This is because we may employ the principle of short time isolation (section 2.1 of Chapter III) and derive in the same way results (2.12) and (3.9) on account of the fact that properties \mathbf{r} , \mathbf{p} and \mathbf{p}' are unaffected during a short enough time during which the fields $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ may be switched off.* The problems of deriving (2.12) and (3.9) with and without the external fields are *similar*, and since only our general knowledge is different, the form of the similarity principle in (5.1.6) of Chapter I applies leaving $\phi_p(\mathbf{r})$, $\phi_r(\mathbf{p})$, $\phi_p(\mathbf{p})$ and $\phi_p(\mathbf{p}')$ unchanged.

5. Implications of the correspondence principle

The passage to the classical limit of particle motion under the action of general (scalar and vector) potentials can be achieved by considering the case of pure knowledge represented in the form of wave packets.†

Using the transformation functions $\phi_p(\mathbf{r})$ and $\phi_r(\mathbf{p})$ and Feynman's law, we note first, using (3.10), that the general relationship between the wave functions $\psi(\mathbf{r}, t)$ and $a(\mathbf{p}, t)$ in the coordinate and momentum representations is

$$\left. \begin{aligned} \psi(\mathbf{r}, t) &= (2\pi\hbar)^{-3/2} \int a(\mathbf{p}, t) \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar) d^3\mathbf{p} \\ a(\mathbf{p}, t) &= (2\pi\hbar)^{-3/2} \int \psi(\mathbf{r}, t) \exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar) d^3\mathbf{r} \end{aligned} \right\} \quad (5.1)$$

i.e. one wave function is always the Fourier transform of the other.

The limit of classical motion of the particle on a definite (classical) orbit is approached by considering the case where $\psi(\mathbf{r}, t)$ and $a(\mathbf{p}, t)$ have significant values only within (classically small) regions of dimensions Δ_r and Δ_p in coordinate and momentum space respectively with

$$\Delta_r \Delta_p \approx \hbar. \quad (5.2)$$

* Note that the first of (3.9) cannot be true if $V(\mathbf{r}, t)$ is infinite in some region of space. As we have said before, a particle cannot enter such a region so $\phi_p(\mathbf{r})$ should be zero there. The method of calculating $\phi_p(\mathbf{r})$ evidently breaks down when $V(\mathbf{r}, t)$ is infinite in some region and exact knowledge of particle momentum is evidently not possible then.

† See section 1 of Chapter XII for the general theory of this.

Case of constant potentials

We first consider particle motion under the action of constant uniform (scalar and vector) potentials V and \mathbf{A} . Substitution of the first of (5.1) into the Schrödinger equation (4.2.4) of Chapter IV shows that the wave function $a(\mathbf{p}, t)$ in momentum space then satisfies the differential equation

$$-\frac{\hbar}{i} \frac{\partial a}{\partial t} = E a$$

where

$$E = \frac{p^2}{2m} - \frac{1}{2\alpha} \gamma V - \frac{1}{m} \mathbf{p} \cdot \mathbf{A} \frac{\varepsilon}{2\alpha} + \frac{A^2}{2m} \frac{\varepsilon^2 - 4\beta\alpha}{2\alpha}. \quad (5.3)$$

The differential equation for $a(\mathbf{p}, t)$ has the solution

$$a(\mathbf{p}, t) = a(\mathbf{p}, 0) e^{-i \frac{E}{\hbar} t}.$$

Hence the first of (5.1) can be rewritten as

$$\psi(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int a(\mathbf{p}, 0) \exp i(\mathbf{p}\mathbf{r} - Et)/\hbar d^3\mathbf{p} \quad (5.4)$$

where E is the function of \mathbf{p} given by (5.3). Let \mathbf{r}_0 and \mathbf{p}_0 mark the centres of the wave packets $\psi(\mathbf{r}, t)$ and $a(\mathbf{p}, t)$. Then, since $\Delta_p \ll p_0$, the integrand in (5.4) is of significant value only for values of \mathbf{p} close to \mathbf{p}_0 and for short enough times t , the phase Et is not much different in (5.4) from the value $E(\mathbf{p}_0)t$. Hence in (5.4) we can put,

$$E = E(\mathbf{p}_0) + (\mathbf{p} - \mathbf{p}_0) \cdot \left. \frac{\partial E}{\partial \mathbf{p}} \right|_{\mathbf{p}=\mathbf{p}_0} \quad (5.5)$$

Using (5.5) in (5.4) amounts to omission of a remainder term of order $(\mathbf{p} - \mathbf{p}_0)^2 t / 2m$ assuming α in (5.3) is of order 1. The condition for omitting this remainder in the exponent of (5.4) is evidently that

$$(\mathbf{p} - \mathbf{p}_0)^2 t / 2m\hbar \ll 1 \quad \text{for} \quad |\mathbf{p} - \mathbf{p}_0| \approx \Delta_p \quad (5.6)$$

and this can hold only for short enough times. Then by (5.5) and (5.3) we have

$$E = E(\mathbf{p}_0) + \left(\frac{\mathbf{p}_0}{m} \frac{1}{2\alpha} - \frac{1}{m} \mathbf{A} \frac{\varepsilon}{2\alpha} \right) \cdot (\mathbf{p} - \mathbf{p}_0). \quad (5.7)$$

Using (5.7) in (5.4) we see that $|\psi(\mathbf{r}, t)|^2$ is a function of $\mathbf{r} - \mathbf{v}_0 t$ (rather than of \mathbf{r} and t separately) where \mathbf{v}_0 is given by

$$\mathbf{v}_0 = \left(\frac{\mathbf{p}_0}{m} \frac{1}{2\alpha} - \frac{1}{m} \mathbf{A} \frac{\varepsilon}{2\alpha} \right). \quad (5.8)$$

Therefore, for short times, the wave packet in coordinate space (or rather its density $|\psi(\mathbf{r}, t)|^2$) simply moves as a whole with this constant (group) velocity, i.e. $|\psi(\mathbf{r}, t)|^2 = f(\mathbf{r} - \mathbf{v}_0 t)$.^{*} This is in agreement with the classical law (Newton's first law of motion) which states that the particle moves uniformly in a straight line when the force on it (i.e. $-\partial\mathbf{A}/\partial t - \nabla V + \mathbf{v}_0 \times (\nabla \times \mathbf{A})$) is zero. But by the correspondence principle we also require, when $\mathbf{A} = 0$, that the momentum \mathbf{p}_0 (being a property with classical analogue) should equal $m\mathbf{v}_0$. By (5.8) this means

$$\alpha = 1/2. \quad (5.9)$$

This establishes the value of α in the Schrödinger equation (4.1.4) of Chapter IV[†]. Using the result $\varepsilon/2\alpha = 1$ found in (5.11) of Chapter IV, (5.8) becomes

$$\mathbf{v}_0 = \frac{\mathbf{p}_0 - \mathbf{A}}{m}.$$

This is in agreement with the classical relation between particle velocity \mathbf{v}_0 and particle *generalised* momentum \mathbf{p}_0 in a uniform electromagnetic vector potential[‡], the potential \mathbf{A} being then $q\mathbf{A}_{\text{em}}/c$ where \mathbf{A}_{em} is the electromagnetic vector potential and q the particle's charge (as in (C.3) of Appendix C where \mathbf{A}_{em} is simply denoted by \mathbf{A}). This

^{*} As we have said this holds true only for times satisfying (5.6). During such times the packet still moves a distance large compared to its size. At a time $t \approx 2m\hbar/\Delta_p^2$, when (5.6) begins to fail, the packet has moved a distance $v_0 t \approx (p_0/m)(2m\hbar/\Delta_p^2) \approx (p_0/\Delta_p)(2\hbar/\Delta_p) \approx (p_0/\Delta_p)\Delta_r$ and this is extremely large compared to Δ_r since $p_0/\Delta_p \gg 1$.

[†] Had we chosen to make $\beta = -1$ (instead of $+1$) at the end of section 2, the particle momentum/momentum and momentum/position transformation functions would have then had to have been the conjugates of the functions we obtained (and which are normally employed). (In fact all wave functions over position or momentum would have then had to have been the conjugates of those we actually employ.) The sign of \mathbf{p} would have been different in (5.3) and that of $\mathbf{p}\cdot\mathbf{r}$ different in (5.4). Therefore the sign of \mathbf{A} would have been different in (5.7). The sign of \mathbf{p}_0 in (5.8) would have changed, and we would have found that the value of α was $-1/2$ rather than $1/2$.

[‡] See, for example, p.49 of [15] where generalised momentum is denoted by \mathbf{P} .

suggests that, at least in the case of a constant uniform electromagnetic vector potential, what we call ‘particle momentum’ \mathbf{p} in quantum mechanics might be the analogue of the classical *generalised* momentum. We will take up this question fully in section 8.

Case of a scalar potential of uniform gradient

We can find the correct value for γ in the Schrödinger equation (4.2.4) of Chapter IV (and hence, through relations (5.11) of Chapter IV, the correct value for β in the same Schrödinger equation) by considering particle motion under the external scalar potential

$$V = -\mathbf{F} \cdot \mathbf{r} \quad (5.10)$$

where \mathbf{F} is a constant which should be identified with the force on the particle in the classical limit.

The Schrödinger equation is now

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \psi = -\gamma V \psi .$$

Substituting (5.10) for V and using the first relation in (5.1) for ψ (on the LHS only) this becomes

$$(2\pi\hbar)^{-3/2} \int \left(-\frac{\hbar}{i} \frac{\partial a}{\partial t} - \frac{p^2}{2m} a \right) \exp(i\mathbf{p} \cdot \mathbf{r} / \hbar) d^3\mathbf{p} = \gamma \mathbf{F} \cdot \mathbf{r} \psi .$$

Taking the inverse Fourier transform gives

$$\begin{aligned} -\frac{\hbar}{i} \frac{\partial a}{\partial t} - \frac{p^2}{2m} a &= (2\pi\hbar)^{-3/2} \int (\gamma \mathbf{F} \cdot \mathbf{r} \psi) \exp(-i\mathbf{p} \cdot \mathbf{r} / \hbar) d^3\mathbf{r} \\ &= -\frac{\hbar}{i} \gamma \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{p}} (2\pi\hbar)^{-3/2} \int \psi \exp(-i\mathbf{p} \cdot \mathbf{r} / \hbar) d^3\mathbf{r} \\ &= -\frac{\hbar}{i} \gamma \mathbf{F} \cdot \frac{\partial a}{\partial \mathbf{p}} \end{aligned}$$

So the differential equation for a is in this case

$$-\frac{\hbar}{i} \left(\frac{\partial a}{\partial t} - \gamma \mathbf{F} \cdot \nabla a \right) = \frac{p^2}{2m} a \quad (5.11)$$

the gradient referring to momentum space.

We now transform our coordinates in momentum space from coordinates O_p employed so far to coordinates O'_p moving at velocity \mathbf{v} ($= -\gamma\mathbf{F}$) relative to O_p .^{*} That is, we put $\mathbf{p} = \mathbf{p}' + \mathbf{v}t$. Then $a'(\mathbf{p}', t)$ in O'_p is related to $a(\mathbf{p}, t)$ in O_p by

$$a(\mathbf{p}, t) = a'(\mathbf{p}', t) \Big|_{\mathbf{p}' = \mathbf{p} - \mathbf{v}t}$$

and we have at any 'event' in momentum space that

$$\begin{aligned} a &= a' \\ \nabla a &= \nabla a' \\ \frac{\partial a}{\partial t} &= \frac{\partial a'}{\partial t} + \frac{\partial a'}{\partial \mathbf{p}'} \cdot \frac{\partial \mathbf{p}'}{\partial t} = \frac{\partial a'}{\partial t} - \mathbf{v} \cdot \nabla a' \end{aligned}$$

the last two relations giving

$$\frac{\partial a}{\partial t} + \mathbf{v} \cdot \nabla a = \frac{\partial a'}{\partial t}.$$

In O'_p (5.11) therefore becomes

$$-\frac{\hbar}{i} \frac{\partial a'}{\partial t} = \frac{(\mathbf{p}' + \mathbf{v}t)^2}{2m} a'$$

with solution

$$a'(\mathbf{p}', t) = a'(\mathbf{p}', 0) e^{-if(\mathbf{p}', t)/\hbar}$$

where

$$\frac{\partial f}{\partial t} = \frac{(\mathbf{p}' + \mathbf{v}t)^2}{2m}, \quad f(\mathbf{p}', 0) = 0$$

or

$$f = \frac{p'^2}{2m} t + \frac{\mathbf{p}' \cdot \mathbf{v}}{2m} t^2 + \frac{v^2}{6m} t^3.$$

So the solution to (5.11) is

^{*} Being a velocity in momentum space, \mathbf{v} has the units of *momentum* per unit time.

$$a(\mathbf{p}, t) = a'(\mathbf{p}', t) \Big|_{\mathbf{p}' = \mathbf{p} - \mathbf{v}t} = a'(\mathbf{p} - \mathbf{v}t, 0) e^{-\frac{i}{\hbar} \left[\frac{(\mathbf{p} - \mathbf{v}t)^2}{2m} t + \frac{(\mathbf{p} - \mathbf{v}t) \cdot \mathbf{v}}{2m} t^2 + \frac{v^2}{6m} t^3 \right]}$$

Substituting this result into the first of (5.1) we obtain

$$\psi(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int a'(\mathbf{p} - \mathbf{v}t, 0) e^{-\frac{i}{\hbar} \left[\frac{(\mathbf{p} - \mathbf{v}t)^2}{2m} t + \frac{(\mathbf{p} - \mathbf{v}t) \cdot \mathbf{v}}{2m} t^2 + \frac{v^2}{6m} t^3 \right]} \exp(i\mathbf{p} \cdot \mathbf{r} / \hbar) d^3\mathbf{p}.$$

Shifting the origin of integration by $\mathbf{v}t$ (i.e. replacing $\mathbf{p} - \mathbf{v}t$ by \mathbf{p}) gives

$$\psi(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int a'(\mathbf{p}, 0) e^{-\frac{i}{\hbar} \left[\frac{p^2}{2m} t + \frac{\mathbf{p} \cdot \mathbf{v}}{2m} t^2 + \frac{v^2}{6m} t^3 \right]} \exp(i\mathbf{p} \cdot \mathbf{r} / \hbar) d^3\mathbf{p} \cdot \exp(i\mathbf{v}t \cdot \mathbf{r} / \hbar). \quad (5.12)$$

Since $a'(\mathbf{p}, 0)$ and $a(\mathbf{p}, 0)$ are the same function of \mathbf{p} we have

$$|\psi(\mathbf{r}, t)|^2 = (2\pi\hbar)^{-3} \left| \int a(\mathbf{p}, 0) \exp[i(\mathbf{p} \cdot \mathbf{r} - g(\mathbf{p}, t)) / \hbar] d^3\mathbf{p} \right|^2 \quad (5.13)$$

where

$$g(\mathbf{p}, t) = \frac{p^2}{2m} t - \gamma \frac{\mathbf{p} \cdot \mathbf{F}}{2m} t^2.$$

Since we are considering a wave packet, $a(\mathbf{p}, 0)$ is very small except when \mathbf{p} is close to \mathbf{p}_0 and in (5.13) we can approximate g thus:

$$g(\mathbf{p}, t) = g(\mathbf{p}_0, t) + (\mathbf{p} - \mathbf{p}_0) \cdot \frac{\partial g}{\partial \mathbf{p}} \Big|_{\mathbf{p} = \mathbf{p}_0} \quad (5.14)$$

So in (5.13)

$$\mathbf{p} \cdot \mathbf{r} - g(\mathbf{p}, t) = \mathbf{p} \cdot \left(\mathbf{r} - \frac{\mathbf{p}_0}{m} t + \frac{1}{2} \gamma \frac{\mathbf{F}}{m} t^2 \right) + \frac{1}{2m} p_0^2 t \quad (5.15)$$

the last term vanishing when we take the modulus squared in (5.13). In making the approximation (5.14) we are again omitting a remainder term of order $(\mathbf{p} - \mathbf{p}_0)^2 t / 2m\hbar$ in the exponent in (5.13) but this, as we said before, can be neglected under condition (5.6).

The form (5.15) for $\mathbf{p} \cdot \mathbf{r} - g(\mathbf{p}, t)$ in (5.13) shows that $|\psi(\mathbf{r}, t)|^2$ is just a function of $\mathbf{r} - \frac{\mathbf{p}_0}{m} t + \frac{1}{2} \gamma \frac{\mathbf{F}}{m} t^2$ so the wave packet in space moves so its centre \mathbf{r}_0 follows the trajectory

$$\mathbf{r}_0 = \frac{\mathbf{p}_0}{m}t - \frac{1}{2}\gamma\frac{\mathbf{F}}{m}t^2.$$

This agrees with the expected classical trajectory only if γ is -1 . And by the relation (5.11) of Chapter IV we have finally found the correct values for all the numerical constants in the Schrödinger equation (4.2.4) of Chapter IV, namely

$$\alpha = 1/2, \quad \gamma = -1, \quad \varepsilon = 1, \quad \beta = 0. \quad (5.16)$$

6. Laws regarding momentum

In the ‘*Case of constant potentials*’ in section 5 we showed that under any pure state of knowledge Y of particle motion in constant potentials the wave function $a(\mathbf{p}, t)$ in the momentum representation has the general form

$$a(\mathbf{p}, t) = a(\mathbf{p}, 0)e^{-\frac{E}{\hbar}t} \quad (6.1)$$

with E given by (5.3). With the values of $\alpha, \gamma, \varepsilon$ and β in (5.16) we have

$$E = \frac{p^2}{2m} + V - \frac{1}{m}\mathbf{p} \cdot \mathbf{A} + \frac{A^2}{2m}. \quad (6.2)$$

where V and \mathbf{A} are constants.

In (6.1) the initial form $a(\mathbf{p}, 0)$ of the wave function is arbitrary and dependent on our pure state of knowledge.

It is clear from (6.1) that our degree of belief distribution $|a(\mathbf{p}, t)|^2$ remains unchanged over time. And this is consistent with the particle momentum itself remaining unchanged. But to show that momentum is actually conserved during motion in a constant scalar and/or vector potential we need to consider the special pure state of knowledge represented by

$$a(\mathbf{p}, 0) = \delta(\mathbf{p} - \mathbf{p}_0) \quad (6.3)$$

In this case we have exact knowledge of the particle momentum at time $t = 0$ and (6.1) gives

$$a(\mathbf{p}, t) = \delta(\mathbf{p} - \mathbf{p}_0)e^{-\frac{E}{\hbar}t} \quad (6.4)$$

Denoting Y by $d^3\mathbf{p}_0$ meaning ‘ \mathbf{p} lies in element $d^3\mathbf{p}_0$ at \mathbf{p}_0 at time $t=0$ ’ we can rewrite (6.4) as

$$\Phi(d^3\mathbf{p} \ t | d^3\mathbf{p}_0 \ 0) = \delta_{d^3\mathbf{p}, d^3\mathbf{p}_0} e^{-i\frac{E}{\hbar}t}$$

from which we have, by the first law of extreme values of probability that $d^3\mathbf{p}_0 \Rightarrow^\alpha d^3\mathbf{p}_0 \ t$ or equivalently $(\mathbf{p}_0, 0) \Rightarrow^\alpha (\mathbf{p}_0, t)$ where α has the determinate value

$$\alpha = -\frac{E}{\hbar}t = -\frac{t}{\hbar} \left[\frac{p_0^2}{2m} + V - \frac{1}{m} \mathbf{p}_0 \cdot \mathbf{A} + \frac{A^2}{2m} \right]$$

So we have the following law.

Conservation of momentum If a particle of mass m moves under the action of constant and uniform scalar and vector potentials V and \mathbf{A} , and has momentum \mathbf{p}_0 at time $t=0$ then this implies, with phase of implication $-\frac{t}{\hbar} \left[\frac{p_0^2}{2m} + V - \frac{1}{m} \mathbf{p}_0 \cdot \mathbf{A} + \frac{A^2}{2m} \right]$, that at any time t the particle’s momentum is \mathbf{p}_0 . Particle momentum is therefore conserved.

This holds quite independently of any knowledge we may or may not have regarding the dynamics of the particle motion. It is a result logically derived from the laws of complex-valued probability and the laws of quantum mechanics.

The law of conservation of momentum under constant uniform V and \mathbf{A} is consistent with the third law of potential action (section 3.2 of Chapter III) which claims that momentum is increased at a rate proportional to the spatial *gradients* of the local potentials. (On the basis of the latter law alone it might be thought possible to deduce (in place of (6.4)) that $a(\mathbf{p}, t) = \delta(\mathbf{p} - \mathbf{p}_0)$ knowing $a(\mathbf{p}, 0) = \delta(\mathbf{p} - \mathbf{p}_0)$. This might be thought to follow from the fact that uniform V and \mathbf{A} produce no change in the momentum over time and that therefore the problems of finding $a(\mathbf{p}, t)$ (given $a(\mathbf{p}, 0) = \delta(\mathbf{p} - \mathbf{p}_0)$) with and without potentials V and \mathbf{A} are *similar*, with similarity relation (5.1.6) of Chapter I applying. But this particular claim of similarity is evidently not valid. When V and \mathbf{A} are changed, knowledge $\mathbf{p} = \mathbf{p}_0$ at time $t=0$ entails knowledge of a change in the energy E of the particle (given by (6.2)). We thus have dissimilar (stationary) states of knowledge (see section 3 of Chapter XI.)

In the ‘*Case of a scalar potential of uniform gradient*’ in section 5 we showed that under any pure state of knowledge Y of particle motion in a scalar potential of uniform gradient the wave function $a(\mathbf{p}, t)$ in the momentum representation has the general form

$$a(\mathbf{p}, t) = a(\mathbf{p} - \mathbf{v}t, 0) e^{-\frac{i}{\hbar} \left[\frac{(\mathbf{p} - \mathbf{v}t)^2}{2m} t + \frac{(\mathbf{p} - \mathbf{v}t) \cdot \mathbf{v}}{2m} t^2 + \frac{v^2}{6m} t^3 \right]} \quad (6.5)$$

where $\mathbf{v} = -\gamma \mathbf{F} = \mathbf{F}$ is the constant in the given potential field

$$V = -\mathbf{F} \cdot \mathbf{r} \quad (6.6)$$

or what would classically be the force acting on the particle. At $t=0$ (6.5) becomes

$$a(\mathbf{p}, t) \Big|_{t=0} = a(\mathbf{p}, 0)$$

so that $a(\mathbf{p}, 0)$ is the wave function at $t=0$ and can be taken to represent our pure state of knowledge Y .

In the particular case in which Y consists in knowing the particle momentum is \mathbf{p}_0 at time $t=0$ we have $a(\mathbf{p}, 0) = \delta(\mathbf{p} - \mathbf{p}_0)$ and therefore by (6.5), putting $\mathbf{v} = \mathbf{F}$,

$$a(\mathbf{p}, t) = \delta(\mathbf{p} - (\mathbf{p}_0 + \mathbf{F}t)) e^{-\frac{i}{\hbar} \left[\frac{p_0^2}{2m} t + \frac{\mathbf{p}_0 \cdot \mathbf{F}}{2m} t^2 + \frac{F^2}{6m} t^3 \right]} \quad (6.7)$$

or

$$\Phi(d^3 \mathbf{p} t | d^3 \mathbf{p}_0 0) = \delta_{d^3 \mathbf{p}, d^3 \mathbf{p}_0} e^{-\frac{i}{\hbar} \left[\frac{p_0^2}{2m} t + \frac{\mathbf{p}_0 \cdot \mathbf{F}}{2m} t^2 + \frac{F^2}{6m} t^3 \right]}$$

where $d^3 \mathbf{p}_0$ is at \mathbf{p}_0 and $d^3 \mathbf{p}$ is at $\mathbf{p}_0 + \mathbf{F}t$. From this we conclude that $d^3 \mathbf{p}_0 0 \Rightarrow^\alpha d^3 \mathbf{p} t$, or $(\mathbf{p}_0, 0) \Rightarrow^\alpha (\mathbf{p}_0 + \mathbf{F}t, t)$ where α has the determinate value

$$\alpha = -\frac{i}{\hbar} \left[\frac{p_0^2}{2m} t + \frac{\mathbf{p}_0 \cdot \mathbf{F}}{2m} t^2 + \frac{F^2}{6m} t^3 \right]. \quad (6.8)$$

This gives us the following law.

Law of momentum increase

If a particle of mass m moves in a scalar potential V of uniform gradient $\nabla V (= -\mathbf{F})$ and has momentum \mathbf{p}_0 at time $t=0$ then this implies, with phase of implication α given in (6.8) that its momentum at time t is $\mathbf{p}_0 + \mathbf{F}t$.

This holds quite independently of any knowledge we may or may not have regarding particle dynamics, and it is consistent with the third law of potential action (in section 3.2 of Chapter III).

Newton's law is thus confirmed in this case but only as a law of *momentum* increase. And momentum is an internal property of the particle and not particle mass m multiplied by particle velocity $\dot{\mathbf{r}}$ since $\dot{\mathbf{r}}$ does not exist. So we cannot conclude that (under the action of the potential (6.6)) particle *position* (as well as particle momentum) changes in time as it would in classical mechanics.*

7. Momentum in a uniformly moving coordinate system

In addition to the property of particle momentum relative to a fixed coordinate system we suppose there is a (vector) property 'particle momentum' relative to any uniformly moving coordinate system O' . This too is an internal property of the particle. And taking a coordinate system O at rest and momentarily coincident with O' at time t , and letting the mass of the particle be m and the velocity of O' be \mathbf{v} , we claim the following law.

Law of momentum in a uniformly moving coordinate system

A particle momentum \mathbf{p} in O at time t implies, with phase of implication zero, a particle momentum $\mathbf{p}' = \mathbf{p} - m\mathbf{v}$ in O' at time t . And conversely a particle momentum \mathbf{p}' in O' at time t implies, with phase of implication zero, a particle momentum $\mathbf{p} = \mathbf{p}' + m\mathbf{v}$ in O at time t .

It follows from this law, as can easily be demonstrated, that the relation (at any one time t) between the momenta of a particle in any two uniformly moving frames of reference (inertial frames) is exactly the same as it would be in classical mechanics. That relation can always be expressed as an implication of one proposition by another with a determinate phase of implication whether or not the inertial frames in question coincide or occupy different positions in space at time t . So that relation necessarily holds true regardless of any knowledge we may or may not hold about the particle motion.

We claim that the property of momentum \mathbf{p}' in O' is a *basic* property. Accordingly there are transformation functions $\phi_{p'}(\mathbf{p})$ and $\phi_p(\mathbf{p}')$ relating wave functions over \mathbf{p} in O at time t and wave functions over \mathbf{p}' in O' at time t when O and O' momentarily coincide.

From the above law of momentum in a uniformly moving coordinate system we can say at once that

$$\phi_p(\mathbf{p}') = \phi_{p'}(\mathbf{p}) = \delta(\mathbf{p} - (\mathbf{p}' + m\mathbf{v})) \quad (7.1)$$

* That such a conclusion does hold in the classical limit does not mean (even in this case) that the (real) increase in quantum mechanical momentum is the *cause* of the expected acceleration. It means only that quantum mechanical momentum and mass \times particle velocity are expected to be *correlated* in the classical limit.

and using Feynman's law we can derive from this the momentum/momentum and momentum/position transformation functions between any pair of inertial frames. First however we will pause to derive the position/position transformation functions in a uniformly moving coordinate system under constant potentials.

7.1 Position/position transformation functions in a uniformly moving coordinate system under constant potentials

Suppose O is at rest and O' moves so that the displacement \mathbf{A} of its origin from that of O is $\mathbf{v}t$. The two coordinate systems then coincide at time $t=0$. By (4.1.18) of Chapter IV the position/position transformation function in O from $\mathbf{r}_1 t_1$ to $\mathbf{r}t$ (without inserting the known values of the constants $\alpha, \varepsilon, \beta$ and γ) is

$$\phi_{\mathbf{r}_1 t_1}(\mathbf{r}t) = \left(\frac{i\pi\hbar}{\alpha m}(t-t_1)\right)^{-3/2} \exp i\left(\frac{\alpha m(\mathbf{r}-\mathbf{r}_1)^2}{\hbar(t-t_1)} + \frac{\varepsilon}{\hbar}\mathbf{A}\cdot(\mathbf{r}-\mathbf{r}_1) + \left(\beta\frac{A^2}{m\hbar} + \gamma\frac{V}{\hbar}\right)(t-t_1)\right). \quad \dots(7.1.1)$$

V and \mathbf{A} being the constant potentials that are assumed to be present. We leave the constants $\alpha, \varepsilon, \beta$ and γ general in order to show that the relations between them established in section 5 of Chapter IV can also be derived by applying the quantum mechanical equivalence principle to the position/position transformation functions in O and O' .

From (7.1.1) we can at once calculate the position/position transformation functions $\phi'_{\mathbf{r}'_1 t_1}(\mathbf{r}'t)$ in O' . We simply use the kinematic (propositional) relations

$$\left. \begin{array}{l} \mathbf{r}t \stackrel{0}{\Leftrightarrow} \mathbf{r}'t \\ \mathbf{r}_1 t_1 \stackrel{0}{\Leftrightarrow} \mathbf{r}'_1 t_1 \end{array} \right\} \quad (7.1.2)$$

when $\mathbf{r} = \mathbf{r}' + \mathbf{v}t$ and $\mathbf{r}_1 = \mathbf{r}'_1 + \mathbf{v}t_1$. These give

$$\phi'_{\mathbf{r}'_1 t_1}(\mathbf{r}'t) = \phi_{\mathbf{r}_1 t_1}(\mathbf{r}t) \Big|_{\substack{\mathbf{r}=\mathbf{r}'+\mathbf{v}t \\ \mathbf{r}_1=\mathbf{r}'_1+\mathbf{v}t_1}}$$

and after some algebra we obtain

$$\begin{aligned} \phi'_{\mathbf{r}'_1 t_1}(\mathbf{r}'t) = & \left(\frac{i\pi\hbar}{\alpha m}(t-t_1)\right)^{-3/2} \exp i\left(\frac{\alpha m(\mathbf{r}'-\mathbf{r}'_1)^2}{\hbar(t-t_1)} + \left(\frac{\varepsilon}{\hbar}\mathbf{A} + \frac{2\alpha m}{\hbar}\mathbf{v}\right)\cdot(\mathbf{r}'-\mathbf{r}'_1) \right. \\ & \left. + \left(\beta\frac{A^2}{m\hbar} + \gamma\frac{V}{\hbar} + \frac{\alpha m}{\hbar}v^2 + \frac{\varepsilon}{\hbar}\mathbf{A}\cdot\mathbf{v}\right)(t-t_1)\right) \end{aligned} \quad \dots(7.1.3)$$

for the required transformation functions in the moving frame.

By the quantum mechanical equivalence principle (section 3.8 of Chapter III) we may instead regard O' to be at rest provided we add $m\mathbf{v}$ to \mathbf{A} and $-\frac{1}{2}mv^2 - \mathbf{v}\cdot\mathbf{A}$ to V to give new constant values \mathbf{A}' and V' of the potentials. When we do that (7.1.3) should return to the original form (7.1.1). That is we should get

$$\begin{aligned} \phi'_{r'_1}(\mathbf{r}'t) = & \left(\frac{i\pi\hbar}{\alpha m}(t-t_1)\right)^{-3/2} \exp i\left(\frac{\alpha m(\mathbf{r}'-\mathbf{r}'_1)^2}{\hbar(t-t_1)} + \frac{\varepsilon}{\hbar}\mathbf{A}'\cdot(\mathbf{r}'-\mathbf{r}'_1)\right. \\ & \left. + \left(\beta\frac{A'^2}{m\hbar} + \gamma\frac{V'}{\hbar}\right)(t-t_1)\right) \end{aligned}$$

This clearly requires that

$$\frac{\varepsilon}{\hbar}\mathbf{A} + \frac{2\alpha m}{\hbar}\mathbf{v} = \frac{\varepsilon}{\hbar}\mathbf{A}'$$

and

$$\beta\frac{A^2}{m\hbar} + \gamma\frac{V}{\hbar} + \frac{\alpha m}{\hbar}v^2 + \frac{\varepsilon}{\hbar}\mathbf{A}\cdot\mathbf{v} = \beta\frac{A'^2}{m\hbar} + \gamma\frac{V'}{\hbar}.$$

Substituting $\mathbf{A}' = \mathbf{A} + m\mathbf{v}$ and $V' = V - \frac{1}{2}mv^2 - \mathbf{v}\cdot\mathbf{A}$ into these conditions and remembering the conditions must hold for any values of V and \mathbf{A} we do indeed obtain the same two relations between $\alpha, \varepsilon, \beta$ and γ as in (5.11) of Chapter IV.

Inserting the known values of the constants $\alpha, \varepsilon, \beta$ and γ in (7.1.3), we obtain for the position/position transformation equations in the uniformly moving coordinate system O' the result

$$\begin{aligned} \phi'_{r'_1}(\mathbf{r}'t) = & \left(\frac{2i\pi\hbar}{m}(t-t_1)\right)^{-3/2} \exp i\left(\frac{m(\mathbf{r}'-\mathbf{r}'_1)^2}{2\hbar(t-t_1)} + \frac{1}{\hbar}(\mathbf{A} + m\mathbf{v})\cdot(\mathbf{r}'-\mathbf{r}'_1) - \frac{1}{\hbar}(V - \frac{1}{2}mv^2 - \mathbf{A}\cdot\mathbf{v})(t-t_1)\right) \\ & \dots(7.1.4) \end{aligned}$$

7.2 Momentum/momentum transformation functions from a rest frame to one in uniform motion

So far we have established the momentum/momentum transformation functions only at the moment that the rest frame and moving frame coincide. Then (7.1) holds. To generalise this we take again coordinates O and O' as in section 7.1 and consider another coordinate system \tilde{O} at rest and momentarily coincident with O' at time t . We may then apply Feynman's law

$$\Phi(d^3\mathbf{p}'|d^3\mathbf{p}') = \sum_{d^3\tilde{\mathbf{p}}} \Phi(d^3\mathbf{p}'|d^3\tilde{\mathbf{p}})\Phi(d^3\tilde{\mathbf{p}}|d^3\mathbf{p}')$$

at time t . This clearly gives the relation

$$\phi_{p'}(\mathbf{p}) = \int \phi_{\tilde{p}}(\mathbf{p}) \phi_{p'}(\tilde{\mathbf{p}}) d^3\tilde{\mathbf{p}}$$

and substituting for $\phi_{\tilde{p}}(\mathbf{p})$ and $\phi_{p'}(\tilde{\mathbf{p}})$ using formulae (2.12) and (7.1) we find

$$\phi_{p'}(\mathbf{p}) = \delta(\mathbf{p} - (\mathbf{p}' + m\mathbf{v})) e^{-i\mathbf{p}\cdot\mathbf{v}t/\hbar} \quad (7.2.1)$$

valid for all t . This is the momentum/momentum transformation function at time t from the uniformly moving frame O' to the rest frame O coincident with O' at time $t=0$. By reciprocity, the momentum/momentum transformation function from the rest frame O to the uniformly moving frame O' is the conjugate of (7.2.1):

$$\phi_p(\mathbf{p}') = \delta(\mathbf{p} - (\mathbf{p}' + m\mathbf{v})) e^{i\mathbf{p}\cdot\mathbf{v}t/\hbar} \quad (7.2.2)$$

7.3 Momentum/position transformation functions in a uniformly moving coordinate system

With respect to the same coordinate systems O and O' employed in section 7.1 and 7.2 we can find the momentum/position transformation functions in the uniformly moving coordinate system O' by applying Feynman's law twice:

$$\Phi(d^3\mathbf{r}' | d^3\mathbf{p}') = \sum_{d^3\mathbf{r} d^3\mathbf{p}} \Phi(d^3\mathbf{r}' | d^3\mathbf{r}) \Phi(d^3\mathbf{r} | d^3\mathbf{p}) \Phi(d^3\mathbf{p} | d^3\mathbf{p}')$$

at a general time t . This gives

$$\phi_{p'}(\mathbf{r}') = \iint \phi_r(\mathbf{r}') \phi_p(\mathbf{r}) \phi_{p'}(\mathbf{p}) d^3\mathbf{r} d^3\mathbf{p}.$$

By the first of (7.1.2) we have $\phi_r(\mathbf{r}') = \delta(\mathbf{r} - (\mathbf{r}' + \mathbf{v}t))$, and substituting for $\phi_p(\mathbf{r})$ and $\phi_{p'}(\mathbf{p})$ using (3.10) and (7.2.1) we find

$$\phi_{p'}(\mathbf{r}') = (2\pi\hbar)^{-3/2} \exp(i(\mathbf{p}' + m\mathbf{v})\mathbf{r}'/\hbar) \quad (7.3.1)$$

and of course $\phi_{p'}(\mathbf{p}')$ is just the conjugate of this:

$$\phi_r(\mathbf{p}') = (2\pi\hbar)^{-3/2} \exp(-i(\mathbf{p}' + m\mathbf{v})\mathbf{r}'/\hbar). \quad (7.3.2)$$

Formulae (7.3.1) and (7.3.2) are the same formulae as (3.10) except that in the former pair the rest frame momentum $\mathbf{p}' + m\mathbf{v}$ must be employed on the RHS rather than the momentum \mathbf{p}' in the frame O' itself.

7.4 Momentum/momentum transformation functions between coordinate systems moving uniformly at the same velocity

We now use the coordinate systems O and O' employed in sections 7.1 to 7.3 and introduce a third coordinate system O'' which may be any coordinate system moving at the same velocity as O' . We also introduce coordinate systems \tilde{O}' and \tilde{O}'' at rest and momentarily coincident with O' and O'' at time t . We find the momentum/momentum transformation functions between O' and O'' by applying Feynman's law:

$$\Phi(d^3\mathbf{p}''|d^3\mathbf{p}') = \sum_{d^3\tilde{\mathbf{p}}'d^3\tilde{\mathbf{p}}''} \Phi(d^3\mathbf{p}''|d^3\tilde{\mathbf{p}}'')\Phi(d^3\tilde{\mathbf{p}}''|d^3\tilde{\mathbf{p}}')\Phi(d^3\tilde{\mathbf{p}}'|d^3\mathbf{p}')$$

at a general time t . This gives

$$\phi_{p'}(\mathbf{p}'') = \iint \phi_{\tilde{p}'}(\mathbf{p}'')\phi_{\tilde{p}''}(\tilde{\mathbf{p}}'')\phi_{p'}(\tilde{\mathbf{p}}')d^3\tilde{\mathbf{p}}''d^3\tilde{\mathbf{p}}'$$

and substituting for $\phi_{\tilde{p}'}(\mathbf{p}'')$ and $\phi_{p'}(\tilde{\mathbf{p}}')$ using (7.1) and for $\phi_{\tilde{p}''}(\tilde{\mathbf{p}}'')$ using (2.12) we find

$$\phi_{p'}(\mathbf{p}'') = \delta(\mathbf{p}' - \mathbf{p}'')e^{i(\mathbf{p}' + m\mathbf{v}) \cdot \mathcal{A}'/\hbar} \quad (7.4.1)$$

where \mathcal{A}' is the (constant) displacement of the origin of O'' from the origin of O' . And of course $\phi_{p'}(\mathbf{p}')$ is just the conjugate of this:

$$\phi_{p'}(\mathbf{p}') = \delta(\mathbf{p}' - \mathbf{p}'')e^{-i(\mathbf{p}' + m\mathbf{v}) \cdot \mathcal{A}'/\hbar}. \quad (7.4.2)$$

Formulae (7.4.1) and (7.4.2) are the same formulae as (2.12) except that (as in the case of the momentum/position transformation functions in section 7.3) the rest frame momentum $\mathbf{p}' + m\mathbf{v}$ must be employed in the exponents on the RHS rather than the momentum \mathbf{p}' in the frame O' .

As in the case of the transformation functions (2.12) and (3.9) in *stationary* coordinate systems, results (7.2.1), (7.3.1) and (7.4.1) (and their inverse (conjugate) forms) hold whether or not scalar and vector potentials are present expressed by general functions $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ in the stationary coordinate system O . This is evident because the transformation functions all refer to one instant in time and because we claim that the momentum \mathbf{p}' in a uniformly moving coordinate system O' is a property amenable to the principle of short time isolation (cf. the argument employed in section 4).

7.5 Schrödinger equation in a uniformly moving coordinate system

Let coordinate system O be at rest and let coordinate system O' move relative to O at constant velocity \mathbf{v} so that the frames O and O' are momentarily coincident at time $t = 0$.

The Schrödinger equation governing the wave function $\psi(\mathbf{r}, t)$ in O for a single particle under a pure state of knowledge Y is, as we have seen

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla \psi + \frac{A^2}{2m} \psi \quad (7.5.1)$$

where $V = V(\mathbf{r}, t)$ and $\mathbf{A} = \mathbf{A}(\mathbf{r}, t)$ are potentials that may be experienced by the particle.

Under the same pure state of knowledge Y our probability density $\psi'(\mathbf{r}', t)$ in O' is related to $\psi(\mathbf{r}, t)$ thus:

$$\psi(\mathbf{r}, t) = \psi'(\mathbf{r} - \mathbf{v}t, t) \quad (7.5.2)$$

because the propositions 'particle at \mathbf{r} in O at time t ' and 'particle at $\mathbf{r}' = \mathbf{r} - \mathbf{v}t$ in O' at time t ' imply one another with phases of implication equal to zero. We therefore have that

$$\frac{\partial \psi}{\partial t} = \frac{\partial \psi'}{\partial t} - \mathbf{v} \cdot \nabla' \psi' \quad (7.5.3)$$

where ∇' is the gradient ($\partial/\partial \mathbf{r}'$) referred to coordinates O' . Since the gradients in O and O' are equal, (7.5.1) and (7.5.3) show us that $\psi'(\mathbf{r}', t)$ satisfies the equation

$$-\frac{\hbar}{i} \left(\frac{\partial \psi'}{\partial t} - \mathbf{v} \cdot \nabla' \psi' \right) = -\frac{\hbar^2}{2m} \nabla'^2 \psi' + V' \psi' + \frac{i\hbar}{m} \mathbf{A}' \cdot \nabla' \psi' + \frac{A'^2}{2m} \psi' \quad (7.5.4)$$

where

$$\begin{aligned} V' &= V'(\mathbf{r}', t) = V(\mathbf{r}' + \mathbf{v}t, t) \\ \mathbf{A}' &= \mathbf{A}'(\mathbf{r}', t) = \mathbf{A}(\mathbf{r}' + \mathbf{v}t, t) \end{aligned} \quad (7.5.5)$$

are the potentials referred to O' rather than O .

Equation (7.5.4) is the required form for the Schrödinger equation in the moving coordinate system. It can be rewritten as

$$-\frac{\hbar}{i} \frac{\partial \psi'}{\partial t} = -\frac{\hbar^2}{2m} \nabla'^2 \psi' + V' \psi' + \frac{i\hbar}{m} (\mathbf{A}' + m\mathbf{v}) \cdot \nabla' \psi' + \frac{A'^2}{2m} \psi' \quad (7.5.6)$$

or as

$$-\frac{\hbar}{i} \frac{\partial \psi'}{\partial t} = -\frac{\hbar^2}{2m} \nabla'^2 \psi' + (V' - \mathbf{v} \cdot \mathbf{A}' - \frac{1}{2} m v^2) \psi' + \frac{i\hbar}{m} (\mathbf{A}' + m\mathbf{v}) \cdot \nabla' \psi' + \frac{(\mathbf{A}' + m\mathbf{v})^2}{2m} \psi' \quad \dots(7.5.7)$$

where the additional terms simply cancel out.

We can say then that the Schrödinger equation in the moving system O' is the usual Schrödinger equation provided we replace the potentials V' and \mathbf{A}' by potentials \tilde{V} and $\tilde{\mathbf{A}}$ given by*

$$\begin{aligned} \tilde{V} &= V' - \mathbf{v} \cdot \mathbf{A}' - \frac{1}{2} m v^2 \\ \tilde{\mathbf{A}} &= \mathbf{A}' + m\mathbf{v} \end{aligned} \quad (7.5.8)$$

In the case of an N particle system, we have seen that the wave function $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ satisfies the N particle Schrödinger equation ((3.2) of Chapter V), i.e.

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i'^2 \psi + V\psi + \sum_{i=1}^N \left(\frac{i\hbar}{m_i} \mathbf{A}_i \cdot \nabla_i \psi + \frac{1}{2m_i} A_i^2 \psi \right) \quad (7.5.9)$$

in O where we have substituted the known values for the constants $\alpha, \gamma, \varepsilon$ and β . It is evident now that the Schrödinger equation for $\psi'(\mathbf{r}'_1, \dots, \mathbf{r}'_N, t)$ in O' will likewise take the form

$$-\frac{\hbar}{i} \frac{\partial \psi'}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i'^2 \psi' + V'\psi' + \sum_{i=1}^N \left(\frac{i\hbar}{m_i} (\mathbf{A}'_i + m_i \mathbf{v}) \cdot \nabla_i' \psi' + \frac{A_i'^2}{2m_i} \psi' \right) \quad (7.5.10)$$

(corresponding to (7.5.6)) where V' and \mathbf{A}'_i are the potentials V and \mathbf{A}_i expressed as functions of $\mathbf{r}'_1, \dots, \mathbf{r}'_N$ and t . We can rewrite (7.5.10) as

$$-\frac{\hbar}{i} \frac{\partial \psi'}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i'^2 \psi' + \tilde{V}\psi' + \sum_{i=1}^N \left(\frac{i\hbar}{m_i} \tilde{\mathbf{A}}_i \cdot \nabla_i' \psi' + \frac{\tilde{A}_i^2}{2m_i} \psi' \right) \quad (7.5.11)$$

(corresponding to (7.5.7)) where

* These are precisely the changes in potentials we will adopt under Galilean transformation (section 9) when we switch to regarding O' (rather than O) to be at rest. But of course we are not actually changing our rest frame here. Nor does the derivation of equations (7.5.7) and (7.5.8) prove the truth of the quantum mechanical principle of equivalence which is an assertion about actual particle motions.

$$\tilde{V} = V' - \sum_{i=1}^N (\mathbf{v} \cdot \mathbf{A}'_i + \frac{1}{2} m_i v^2) \quad (7.5.12)$$

$$\tilde{\mathbf{A}}_i = \mathbf{A}'_i + m_i \mathbf{v}$$

are replacement potentials -a replacement system potential \tilde{V} and replacement external vector potentials $\tilde{\mathbf{A}}_i$ for each particle.

8. The kinetic momentum and the quantum mechanical velocity of a particle

We noted in the *Case of constant potentials* in section 5, that the velocity \mathbf{v}_0 of a quasi-classical wave packet representing our knowledge of a particle's motion in a fixed coordinate system under a constant vector potential \mathbf{A} is given by

$$\mathbf{v}_0 = \frac{\mathbf{p}_0 - \mathbf{A}}{m} \quad (8.1)$$

where m is the particle mass, \mathbf{p}_0 its momentum (to classical accuracy) and \mathbf{A} the vector potential (electromagnetic or otherwise). Here $m\mathbf{v}_0 (= \mathbf{p}_0 - \mathbf{A})$ is of course the classical (kinetic) momentum of the particle (as opposed to its classical generalised momentum).

We now claim that in the presence of *any* particle vector potential $\mathbf{A}(\mathbf{r}, t)$ and at any time t , the quantum mechanical momentum \mathbf{p} of a particle relative to a stationary coordinate system \mathbf{O} is the analogue of the corresponding classical generalised particle momentum. We claim it is an internal property of the particle made up of the sum of two components, each component having its own classical analogue. One component we will denote by \mathbf{p} and called the 'kinetic momentum' of the particle relative to \mathbf{O} and the other component arises from and is equal (in magnitude and direction) to the value of the net particle vector potential at the position occupied by the particle at time t . The kinetic momentum relative to \mathbf{O} is an internal property of the particle proportional to its mass. The vector quantity \mathbf{p}/m is of course also an internal property of the particle and we call it the 'quantum mechanical velocity' of the particle relative to coordinate system \mathbf{O} . Since a particle does not move smoothly in space we cannot claim the quantum mechanical velocity is the rate of change of the particle position vector in \mathbf{O} because this rate of change does not exist, but the quantum mechanical velocity is nonetheless *classified* as a property of particle orbital motion just as momentum is. It is moreover classified as a *kinematic* property of particle orbital motion. Let $\mathbf{A}(\mathbf{r}, t)$ be the vector potential field as a function of time t and position \mathbf{r} in \mathbf{O} . The field $\mathbf{A}(\mathbf{r}, t)$ acts instantly on the internal motion of the particle giving rise to an extra component of the particle's momentum. So at any time t we have for the momentum \mathbf{p} in \mathbf{O} the relation

$$\mathbf{p} = \mathbf{p} + \mathbf{A}(\mathbf{r}, t) \quad (8.2)$$

where \mathbf{r} is the position in O occupied by the particle at time t .

A relation of the form (8.2) is supposed to hold in any fixed coordinate system, regardless of any knowledge we may or may not hold in relation to the particle motion.

If at time t and relative to some fixed frame O , we know the momentum \mathbf{p} to quantum mechanical accuracy, we cannot generally claim to know also the kinetic momentum \mathbf{p} at time t because in (8.2) we are uncertain of the particle's position \mathbf{r} . We do however know the probability distribution $\psi(\mathbf{r}, t)$ or the wave function in O . By (3.9) it is $(2\pi\hbar)^{-3/2} \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar)$. We therefore have a uniform degree of belief distribution for particle position \mathbf{r} in O , and on the basis of this we are able to calculate a degree of belief distribution over the possible values of $\mathbf{A}(\mathbf{r}, t)$ and thus obtain a degree of belief distribution over \mathbf{p} at time t . In the simple case in which $\mathbf{A}(\mathbf{r}, t)$ is uniform in space (i.e. of the form $\mathbf{A}(\mathbf{r}, t) = \mathbf{A}(t)$) we know immediately (from (8.2)) the value of \mathbf{p} at time t when we know \mathbf{p} at time t .

We have claimed in section 4 that particle momentum relative to a fixed coordinate system is a dynamical property amenable to the principle of short time isolation (stated in section 2.1 of Chapter III). Thus if vector potential $\mathbf{A}(\mathbf{r}, t)$ is 'switched off' (or suddenly changed) at time t no sudden change in \mathbf{p} occurs. Owing to the general relation (8.2) this implies that the kinetic momentum \mathbf{p} must undergo a sudden change (equal and opposite to the change in $\mathbf{A}(\mathbf{r}, t)$) when $\mathbf{A}(\mathbf{r}, t)$ is 'switched off' or changes suddenly in any way.

The fact that \mathbf{p} is changed but \mathbf{p} is not is consistent with quasi-classical wave packet motion (or classical particle motion) to which Newton's law

$$m\dot{\mathbf{v}}_p = -\partial\mathbf{A}/\partial t - \nabla V + \mathbf{v}_p \times (\nabla \times \mathbf{A}) \quad (8.3)$$

applies in the rest frame (as claimed at the end of section 1 of Chapter III), \mathbf{v}_p being the velocity of the wave packet (or of the classical particle) and the RHS of (8.3) being evaluated at the location \mathbf{r} of the particle. In (8.3) $m\mathbf{v}_p$ is the classical kinetic momentum of the particle (the classical analogue of the quantum mechanical kinetic momentum). And, on account of the term $\partial\mathbf{A}/\partial t$ in (8.3), $m\mathbf{v}_p$ must change abruptly when $\mathbf{A}(\mathbf{r}, t)$ increases by $\Delta\mathbf{A}(\mathbf{r}, t)$ suddenly at time t , the increase $\Delta(m\mathbf{v}_p)$ in $m\mathbf{v}_p$ being given by

$$\begin{aligned} \Delta(m\mathbf{v}_p) &= \lim_{\Delta t \rightarrow 0} \int_t^{t+\Delta t} (-\partial\mathbf{A}/\partial t - \nabla V + \mathbf{v}_p \times (\nabla \times \mathbf{A})) dt = \lim_{\Delta t \rightarrow 0} \int_t^{t+\Delta t} (-\partial\mathbf{A}/\partial t) dt \\ &= -\lim_{\Delta t \rightarrow 0} (\mathbf{A}(\mathbf{r}, t + \Delta t) - \mathbf{A}(\mathbf{r}, t)) = -\Delta\mathbf{A}(\mathbf{r}, t) \end{aligned}$$

(In the case of a charged particle in an electromagnetic field this sudden change in momentum is due to the impulsive action of the electric field induced by the sudden change in the magnetic field or its vector potential.) On the other hand, since

$\dot{\mathbf{A}} = \partial \mathbf{A} / \partial t + (\mathbf{v}_p \cdot \nabla) \mathbf{A}$, the rate of change of the classical *generalised* momentum $m\mathbf{v}_p + \mathbf{A}$ is, by (8.3),

$$m\dot{\mathbf{v}}_p + \dot{\mathbf{A}} = -\nabla V + \mathbf{v}_p \times (\nabla \times \mathbf{A}) + (\mathbf{v}_p \cdot \nabla) \mathbf{A}. \quad (8.4)$$

So we see that generalised momentum $m\mathbf{v}_p + \mathbf{A}$ does *not* change suddenly under a sudden change in $\mathbf{A}(\mathbf{r}, t)$.*

Note that the RHS of (8.4), which might also be considered equal to (or related to) the rate of increase of the *quantum mechanical* momentum of the particle, is of a form consistent with the claims made in the third law of potential action. That is, it is proportional to the first spatial derivatives of V and \mathbf{A} at the position momentarily occupied by the particle.

Finally we make some more claims regarding kinematic properties at any one time t .

We have noted in section 7 that the relation at any one time t between the quantum mechanical momenta of a particle in any two *uniformly moving* coordinate systems is the same as it would be in classical mechanics whatever the velocities of each frame relative to fixed space, whatever positions the frames may occupy at time t and whatever our knowledge of the particle motion might be.

We now claim that the same is true of the quantum mechanical kinetic momenta of a particle (and therefore of the quantum mechanical velocities also). That is, the relation at any one time t between the kinetic momenta of a particle in any two inertial frames is the same as it would be in classical mechanics whatever the velocities of each frame relative to fixed space, whatever positions the frames may occupy at time t and whatever our knowledge of the particle motion might be. In this case however it may not be that the phase of implication in a statement claiming a kinetic momentum in one inertial frame implies the classically related value in another has a determinate value. But we nonetheless claim that statement to be true whatever our knowledge of the particle motion might be.

9. Galilean invariance in quantum mechanics

In the conventional interpretation of quantum mechanics Galilean invariance is accounted for in the way reproduced (for single particle motion) in section 9.1 below. And we give in section 9.1 the conventional Galilean transformation equations and show how these can be brought into line with those of the present interpretation derived in section 9.2 using the quantum mechanical principle of equivalence (section 3.8 of Chapter III). The Galilean transformation equations to be adopted for a many particle system are given in section 9.3.

For the purpose of discussion we employ the same pair of (inertial frame) coordinates O and O' set up in section 5 of Chapter IV where O' moves relative to O at velocity \mathbf{v} , the frames O and O' being momentarily coincident at time $t = 0$.

* cf. the like-minded discussion on p21-5 of [7]

9.1 Galilean invariance in the conventional interpretation of quantum mechanics

Taking O' to be at rest, any wave function $\psi'(\mathbf{r}', t)$ in O' satisfies the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi'}{\partial t} = -\frac{\hbar^2}{2m} \nabla'^2 \psi' + V \psi' + \frac{i\hbar}{m} \mathbf{A}' \cdot \nabla' \psi' + \frac{A'^2}{2m} \psi' \quad (9.1.1)$$

where $\nabla' \equiv \partial/\partial \mathbf{r}'$, and V' and \mathbf{A}' are the potentials expressed in (9.1.1) as functions $V'(\mathbf{r}', t)$ and $\mathbf{A}'(\mathbf{r}', t)$ of the position coordinate in O' and the time, $\nabla' \cdot \mathbf{A}'$ being zero. The sources of the potentials are as seen in the rest frame O' . (In the conventional interpretation there are no ‘background fields’ and hence no components of the potentials due to background fields.)

When taking O to be at rest instead of O' no measurable difference should result. In particular our expectations of the relative frequencies of position measurement outcomes should remain the same so the squared modulus of the wave function $\psi(\mathbf{r}, t)$ in O for the same physical process must equal $|\psi'(\mathbf{r} - \mathbf{v}t, t)|^2$ and in the conventional account of Galilean invariance $\psi(\mathbf{r}, t)$ is claimed to be

$$\psi(\mathbf{r}, t) = \psi'(\mathbf{r} - \mathbf{v}t, t) e^{\frac{i}{\hbar} [m\mathbf{v} \cdot \mathbf{r} - (\frac{1}{2} m v^2) t]} \quad (9.1.2)$$

since this satisfies the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla \psi + \frac{A^2}{2m} \psi \quad (9.1.3)$$

in O where the potentials, expressed by the functions $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ in (9.1.3), are

$$\begin{aligned} V(\mathbf{r}, t) &= V'(\mathbf{r} - \mathbf{v}t, t) + \mathbf{v} \cdot \mathbf{A}'(\mathbf{r} - \mathbf{v}t, t) \\ \mathbf{A}(\mathbf{r}, t) &= \mathbf{A}'(\mathbf{r} - \mathbf{v}t, t) \end{aligned} \quad (9.1.4)$$

on account of the fact that the sources of the potentials now have a velocity (or extra velocity) \mathbf{v} relative to fixed space (i.e. relative to O).

The proof that $\psi(\mathbf{r}, t)$ satisfies (9.1.3) may be conducted by substituting (9.1.2) and (9.1.4) into (9.1.3) and showing (9.1.3) reduces to the original Schrödinger equation (9.1.1) in $\psi'(\mathbf{r}', t)$ which is satisfied by assumption. To carry out the proof we abbreviate $[m\mathbf{v} \cdot \mathbf{r} - (\frac{1}{2} m v^2) t]$ to $[]$, and note that (9.1.2) implies

$$\nabla\psi = e^{\frac{i}{\hbar}[\dots]} \nabla'\psi' + \psi' \nabla e^{\frac{i}{\hbar}[\dots]} = (\nabla'\psi' + \frac{i}{\hbar} m\mathbf{v}\psi') e^{\frac{i}{\hbar}[\dots]}$$

and that therefore

$$\begin{aligned} \nabla^2\psi &= e^{\frac{i}{\hbar}[\dots]} \nabla \cdot (\nabla'\psi' + \frac{i}{\hbar} m\mathbf{v}\psi') + (\nabla'\psi' + \frac{i}{\hbar} m\mathbf{v}\psi') \cdot \nabla e^{\frac{i}{\hbar}[\dots]} \\ &= (\nabla'^2\psi' + 2\frac{i}{\hbar} m\mathbf{v} \cdot \nabla'\psi' - \frac{1}{\hbar^2} m^2 v^2 \psi') e^{\frac{i}{\hbar}[\dots]} \end{aligned}$$

and also

$$\frac{\partial\psi}{\partial t} = \left(\frac{\partial\psi'}{\partial t} - \mathbf{v} \cdot \nabla'\psi' + \psi' \frac{i}{\hbar} \left(-\frac{1}{2} m v^2\right) \right) e^{\frac{i}{\hbar}[\dots]}.$$

All of these consequences of (9.1.2) are relations between derivatives of $\psi(\mathbf{r}, t)$ and the values and derivatives of $\psi'(\mathbf{r}', t)$ when $\mathbf{r}' = \mathbf{r} - \mathbf{v}t$, i.e. at one and the same 'event' in classical space/time. Using these results we easily see that (9.1.3) reduces to the Schrödinger equation (9.1.1).

The momentum wave functions $a(\mathbf{p}, t)$ and $a'(\mathbf{p}', t)$ corresponding to $\psi(\mathbf{r}, t)$ in O and $\psi'(\mathbf{r}', t)$ in O' respectively are, by (5.1),

$$\left. \begin{aligned} a(\mathbf{p}, t) &= (2\pi\hbar)^{-3/2} \int \psi(\mathbf{r}, t) \exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar) d^3\mathbf{r} \\ a'(\mathbf{p}', t) &= (2\pi\hbar)^{-3/2} \int \psi'(\mathbf{r}', t) \exp(-i\mathbf{p}'\cdot\mathbf{r}'/\hbar) d^3\mathbf{r}' \end{aligned} \right\} \quad (9.1.5)$$

and by (9.1.2), $a(\mathbf{p}, t)$ can be written

$$a(\mathbf{p}, t) = (2\pi\hbar)^{-3/2} \int \psi'(\mathbf{r} - \mathbf{v}t, t) e^{\frac{i}{\hbar}[m\mathbf{v}\cdot\mathbf{r} - (\frac{1}{2}m v^2)t]} \exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar) d^3\mathbf{r}$$

which with the substitution $\mathbf{r}' = \mathbf{r} - \mathbf{v}t$ gives

$$\begin{aligned} a(\mathbf{p}, t) &= (2\pi\hbar)^{-3/2} \int \psi'(\mathbf{r}', t) e^{\frac{i}{\hbar}[m\mathbf{v}\cdot(\mathbf{r}'+\mathbf{v}t) - (\frac{1}{2}m v^2)t]} \exp(-i\mathbf{p}\cdot(\mathbf{r}'+\mathbf{v}t)/\hbar) d^3\mathbf{r}' \\ &= (2\pi\hbar)^{-3/2} e^{\frac{i}{\hbar}[m v^2 t - (\frac{1}{2}m v^2)t]} e^{-i\mathbf{p}\cdot\mathbf{v}t/\hbar} \int \psi'(\mathbf{r}', t) \exp(-i(\mathbf{p} - m\mathbf{v})\cdot\mathbf{r}'/\hbar) d^3\mathbf{r}' \end{aligned}$$

We thus obtain the relation

$$a(\mathbf{p}, t) = e^{\frac{i}{\hbar}(\frac{1}{2}m v^2 - \mathbf{p}\cdot\mathbf{v})t} a'(\mathbf{p} - m\mathbf{v}, t)$$

between the corresponding momentum wave functions.

This completes our account of quantum mechanical Galilean invariance as usually given.

We note that under this Galilean invariance the wave functions over position are related (by (9.1.2)) in a manner different from the simple relation $\psi(\mathbf{r}, t) = \psi'(\mathbf{r} - \mathbf{v}t, t)$ which we might expect. Staying within the conventional interpretation of quantum mechanics we may however obtain this simple relation by applying a certain gauge transformation in addition to the transformation (9.1.2) and (9.1.4). A gauge transformation is (in the conventional interpretation of quantum mechanics) allowed as it has no effect on the predicted frequencies of measurement results.

The general gauge transformation in \mathcal{O} is

$$\left. \begin{aligned} V &\rightarrow \tilde{V} = V - \frac{\partial f}{\partial t} \\ \mathbf{A} &\rightarrow \tilde{\mathbf{A}} = \mathbf{A} + \nabla f \\ \psi(\mathbf{r}, t) &\rightarrow \tilde{\psi}(\mathbf{r}, t) = \psi(\mathbf{r}, t) e^{\frac{i}{\hbar} f} \end{aligned} \right\} \quad (9.1.6)$$

where f is any function of \mathbf{r} and t except that as we need to preserve $\nabla \cdot \mathbf{A} = 0$ we must impose the condition $\nabla^2 f = 0$. The transformation (9.1.6) then always results in $\tilde{\psi}(\mathbf{r}, t)$ satisfying the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \tilde{\psi}}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \tilde{\psi} + \tilde{V} \tilde{\psi} + \frac{i\hbar}{m} \tilde{\mathbf{A}} \cdot \nabla \tilde{\psi} + \frac{A^2}{2m} \tilde{\psi}$$

when $\psi(\mathbf{r}, t)$ satisfies the Schrödinger equation (9.1.3).

With the choice $f = -m\mathbf{v} \cdot \mathbf{r} + \frac{1}{2} m\mathbf{v}^2 t$ for the gauge transformation to be added to the usual Galilean transformation (9.1.2) and (9.1.4) we can evidently remove the phase factor in (9.1.2). We thus obtain a ‘new’ Galilean transformation expressed by

$$\psi(\mathbf{r}, t) = \psi'(\mathbf{r} - \mathbf{v}t, t) \quad (9.1.7)$$

and

$$\begin{aligned} V(\mathbf{r}, t) &= V'(\mathbf{r} - \mathbf{v}t, t) + \mathbf{v} \cdot \mathbf{A}'(\mathbf{r} - \mathbf{v}t, t) - \frac{1}{2} m\mathbf{v}^2 \\ \mathbf{A}(\mathbf{r}, t) &= \mathbf{A}'(\mathbf{r} - \mathbf{v}t, t) - m\mathbf{v} \end{aligned} \quad (9.1.8)$$

instead of (9.1.2) and (9.1.4). This is formally the same as the transformation we adopt in *our* interpretation of quantum mechanics (derived in section 9.2). It clearly ensures that $\psi(\mathbf{r}, t)$ satisfies the Schrödinger equation (9.1.3) (where V and \mathbf{A} are given by (9.1.8)) whenever $\psi'(\mathbf{r}', t)$ satisfies the Schrödinger equation (9.1.1).

Corresponding to (9.1.7) the wave functions in the momentum representation are now related by

$$a(\mathbf{p}, t) = e^{-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{v} t} a'(\mathbf{p}, t). \quad (9.1.9)$$

as may easily be checked.

9.2 Galilean invariance in the present interpretation of quantum mechanics

In the present interpretation of quantum mechanics we employ the ‘new’ Galilean transformation equations (9.1.7) and (9.1.8) (and therefore (9.1.9) also). And we show (i) how to establish these equations more directly and (ii) why they represent the most natural way of formulating the Galilean transformation equations.

Our pure knowledge Y regarding the particle motion must always be knowledge of particle dynamical variables expressed relative to O or to O' or to some other coordinate system.

Let $V'(\mathbf{r}', t)$ and $A'(\mathbf{r}', t)$ be the particle potentials in O' when O' is taken as the rest frame. We then have

$$\begin{aligned} V'(\mathbf{r}', t) &= \tilde{V}'(\mathbf{r}', t) + mV'_0 \\ A'(\mathbf{r}', t) &= \tilde{A}'(\mathbf{r}', t) + mA'_0 \end{aligned}$$

where \tilde{V}' and \tilde{A}' are the potentials due to sources, and V'_0 and A'_0 are the constant background potentials.

When we change our choice of rest frame from O' to O it is, on account of the quantum mechanical principle of equivalence, natural to add $-\frac{1}{2}mv^2 + m\mathbf{v} \cdot \mathbf{A}'_0$ and $-m\mathbf{v}$ respectively to the background scalar and vector potentials and we must of course take account of the changed velocity of the sources. We thus arrive at the potentials $V(\mathbf{r}, t)$ and $A(\mathbf{r}, t)$ in O given by (9.1.8). Then, by the quantum mechanical principle of equivalence, the possible particle motions (relative to O or O' or to any other coordinate system) remain the same. And the problem of calculating the probability $\psi(\mathbf{r}, t)$ of one or other event (\mathbf{r}, t) in O under knowledge Y is *similar* to that of calculating the probability $\psi'(\mathbf{r}', t)$ of the same event (\mathbf{r}', t) in O' under the same knowledge Y before our change in mind regarding the rest frame and background potentials. Hence, by the similarity principle ((5.1.6) of Chapter I*), we must have

* We note that although our knowledge Y is the same for wave functions $\psi(\mathbf{r}, t)$ and $\psi'(\mathbf{r}', t)$, and although (\mathbf{r}, t) and (\mathbf{r}', t) refer to one and the same event, our general knowledge is different because of the difference in assumed rest frame and background potentials in each case. Note that were we to adopt a different change in background potentials (on changing our rest frame from O' to O) the quantum mechanical principle of equivalence would not apply and particle motions would likely be different in each case, and *similarity* would no longer be present.

$$\psi(\mathbf{r}, t) = \psi'(\mathbf{r}', t)$$

when $\mathbf{r}' = \mathbf{r} - \mathbf{v}t$. This is the reason it is natural to adopt (9.1.7) and (9.1.8) as our Galilean transformation equations.

As noted in section 9.1 these transformation equations ((9.1.7) and (9.1.8)) ensure that $\psi(\mathbf{r}, t)$ satisfies the Schrödinger equation (9.1.3) (where V and \mathbf{A} are given by (9.1.8)) whenever $\psi'(\mathbf{r}', t)$ satisfies the Schrödinger equation (9.1.1).

This completes the derivation of the Galilean (single particle) transformation equations in the present interpretation of quantum mechanics.

A result (as noted in (9.1.9)) of the Galilean transformation equations is the relation

$$a(\mathbf{p}, t) = e^{-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{v}t} a'(\mathbf{p}, t) \quad (9.2.1)$$

between the corresponding momentum wave functions. When $t = 0$ this reduces to

$$a(\mathbf{p}, 0) = a'(\mathbf{p}, 0). \quad (9.2.2)$$

So the distributions over momentum (before and after our change in choice of the rest frame) are the same at the moment \mathbf{O} and \mathbf{O}' coincide despite their relative motion. This is consistent with the fact that particle momentum includes a contribution arising from the vector potential at the point occupied by the particle, and while the kinetic momentum increases by $m\mathbf{v}$ on change of rest frame from \mathbf{O}' to \mathbf{O} the vector potential increases by an equal and opposite amount.

Finally we note that the presence of the phase factor $e^{-i\mathbf{p} \cdot \mathbf{v}t/\hbar}$ in (9.2.1) needed when $t \neq 0$ simply reflects the fact that at any time $t \neq 0$, \mathbf{O}' is displaced from \mathbf{O} by a distance $\mathbf{A} = \mathbf{v}t$. To see this we derive (9.2.1) assuming the truth of (9.2.2).

First note that (9.2.2) implies

$$\tilde{a}(\mathbf{p}, t) = a'(\mathbf{p}, t). \quad (9.2.3)$$

where $\tilde{a}(\tilde{\mathbf{p}}, t)$ is the momentum wave function referred to an inertial frame $\tilde{\mathbf{O}}$ stationary with respect to \mathbf{O} and momentarily coincident with \mathbf{O}' at time t . Second, working under the assumption that \mathbf{O} is at rest we have, from the first of (2.12), the following propositional relationship at time t .

$$(\tilde{\mathbf{p}} \text{ in } \tilde{\mathbf{O}})^{-\alpha_p} \Leftrightarrow^{\alpha_p} (\mathbf{p} = \tilde{\mathbf{p}} \text{ in } \mathbf{O})$$

where $\alpha_p = -\mathbf{p} \cdot \mathbf{A}/\hbar$ and $\mathbf{A} = \mathbf{v}t$. And since \mathbf{p} in \mathbf{O} and $\tilde{\mathbf{p}}$ in $\tilde{\mathbf{O}}$ are equivalent bases we may apply the general rule (10.2.4) of Chapter II getting

$$\tilde{a}(\mathbf{p}, t) = a(\mathbf{p}, t) e^{i\mathbf{p} \cdot \mathbf{A}/\hbar}. \quad (9.2.4)$$

Replacing $\tilde{a}(\mathbf{p}, t)$ by $a'(\mathbf{p}, t)$ (using (9.2.3)) we obtain (9.2.1). QED.

Taking O to be at rest, the position/momentum transformation function in O is, by (3.10), $\phi_r(\mathbf{p}) = (2\pi\hbar)^{-3/2} \exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar)$. Then, if our pure knowledge regarding particle motion is represented by a general wave function $\psi(\mathbf{r}, t)$ in O , our wave function $a(\mathbf{p}, t)$ in the momentum space corresponding to O is

$$a(\mathbf{p}, t) = (2\pi\hbar)^{-3/2} \int \psi(\mathbf{r}, t) \exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar) d^3\mathbf{r}, \quad (9.2.5)$$

while if we take O' to be at rest, the position/momentum transformation function in the uniformly moving system O is, by (7.3.2), $\phi_r(\mathbf{p}) = (2\pi\hbar)^{-3/2} \exp(-i(\mathbf{p} - m\mathbf{v})\cdot\mathbf{r}/\hbar)$, where the sign of \mathbf{v} is changed on account of O moving at velocity $-\mathbf{v}$ with respect to O' . Our wave function in the momentum space corresponding to O is now

$$(2\pi\hbar)^{-3/2} \int \psi(\mathbf{r}, t) \exp(-i(\mathbf{p} - m\mathbf{v})\cdot\mathbf{r}/\hbar) d^3\mathbf{r}. \quad (9.2.6)$$

and by (9.2.5) is therefore given by

$$a(\mathbf{p} - m\mathbf{v}, t) \quad (9.2.7)$$

so our knowledge regarding particle momentum in O changes even though our knowledge regarding particle position in O (expressed by the wave function $\psi(\mathbf{r}, t)$) does not. But when O is taken to be at rest the *kinetic* momentum in O is, by (8.2)

$$\mathbf{p} = \mathbf{p} - \mathbf{A}(\mathbf{r}, t) \quad (9.2.8)$$

while the kinetic momentum in O when O' is taken to be at rest is

$$\mathbf{p} = \mathbf{p} - (\mathbf{A}(\mathbf{r}, t) + m\mathbf{v}) = (\mathbf{p} - m\mathbf{v}) - \mathbf{A}(\mathbf{r}, t) \quad (9.2.9)$$

because, by the Galilean transformation established above, the vector potential must now be increased by $m\mathbf{v}$. Hence, as we would expect, our kinetic knowledge (our knowledge regarding \mathbf{r} and \mathbf{p} in O over time) is the same whether O or O' is taken to be at rest. In either case the distributions $\psi(\mathbf{r}, t)$ and $a(\mathbf{p} + \mathbf{A}(\mathbf{r}, t), t)$ expressing our knowledge of \mathbf{r} and \mathbf{p} in O are the same.

9.3 Galilean invariance in the case of a many particle system

The generalisation of our Galilean transformation equations (9.1.7) and (9.1.8) to the case of a many particle system is straightforward.

For a system of N distinguishable particles any wave function in configuration space satisfies the Schrödinger equation (3.2) of Chapter V. This means that a wave function $\psi'(\mathbf{r}'_1, \dots, \mathbf{r}'_N, t)$ satisfies

$$-\frac{\hbar}{i} \frac{\partial \psi'}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i'^2 \psi' + V' \psi' + \sum_{i=1}^N \left(\frac{i\hbar}{m_i} \mathbf{A}'_i \cdot \nabla_i' \psi' + \frac{A_i'^2}{2m_i} \psi' \right) \quad (9.3.1)$$

in O' when O' is taken to be at rest. Here m_i is the mass of the i^{th} particle, $V = V'(\mathbf{r}'_1, \dots, \mathbf{r}'_N, t)$ the system potential and $\mathbf{A}'_i = \mathbf{A}'_i(\mathbf{r}'_i, t)$ the external vector potential for the i^{th} particle.

Given the same state of pure knowledge Y of the dynamical properties of the particle motion (relative to O or to O' or any other coordinate system) we require (for the same reasons as those given in section 9.2 for single particle case) that the relation

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t) = \psi'(\mathbf{r}_1 - \mathbf{v}t, \dots, \mathbf{r}_N - \mathbf{v}t, t) \quad (9.3.2)$$

holds between the wave functions in O and O' when respectively O and O' are taken to be at rest. And on account of the change in absolute motion of the sources of potentials and of the need for a change in the background fields, we have, for the potentials in the case when O is taken to be at rest the equations

$$V = V'(\mathbf{r}_1 - \mathbf{v}t, \dots, \mathbf{r}_N - \mathbf{v}t, t) + \sum_{i=1}^N \mathbf{v} \cdot \mathbf{A}'_i(\mathbf{r}_1 - \mathbf{v}t, \dots, \mathbf{r}_N - \mathbf{v}t, t) - \sum_{i=1}^N \frac{1}{2} m_i v^2 \quad (9.3.3)$$

$$\mathbf{A}_i = \mathbf{A}'_i(\mathbf{r}_1 - \mathbf{v}t, \dots, \mathbf{r}_N - \mathbf{v}t, t) - m_i \mathbf{v}$$

which is the generalisation of (9.1.8).

It is demonstrable that $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ then satisfies the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 \psi + V \psi + \sum_{i=1}^N \left(\frac{i\hbar}{m_i} \mathbf{A}_i \cdot \nabla_i \psi + \frac{A_i^2}{2m_i} \psi \right) \quad (9.3.4)$$

in O when O is taken to be at rest and, V and \mathbf{A} are given by (9.3.3).

From (9.3.2) we can show that with first frame O then frame O' taken at rest the wave function $a(\mathbf{p}_1, \dots, \mathbf{p}_N, t)$ in the momentum space of O in the first case given by

$$a(\mathbf{p}_1, \dots, \mathbf{p}_N, t) = (2\pi\hbar)^{-3N/2} \int \dots \int \psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t) \exp(-i(\mathbf{p}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{p}_N \cdot \mathbf{r}_N)/\hbar) d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N \quad \dots(9.3.5)$$

is related to the momentum wave function $a'(\mathbf{p}'_1, \dots, \mathbf{p}'_N, t)$ of O' in the second case by

$$a(\mathbf{p}_1, \dots, \mathbf{p}_N, t) = a'(\mathbf{p}_1, \dots, \mathbf{p}_N, t) e^{-\frac{i}{\hbar} \sum_{i=1}^N \mathbf{p}_i \cdot \mathbf{v}t} \quad (9.3.6)$$

which is the generalisation of (9.1.9). With $t=0$ this relation too is as we expect when we consider that the kinetic momentum of the i^{th} particle increases by $m_i \mathbf{v}$ while its vector potential increases by $-m_i \mathbf{v}$ on change of rest frame from O' to O . And with $t \neq 0$ the phase factor in (9.3.6) again arises because of the relative displacement (by $\mathbf{v}t$) of O' in relation to O .

10. The meaning of gauge invariance

In the usual interpretation of quantum mechanics gauge invariance refers to the possibility of certain alternative representations of physical states. Thus, if the evolving physical state of a single particle moving under the action of potentials $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ is represented by a wave function $\psi(\mathbf{r}, t)$ it is regarded as equally true that the *same evolving state* can be represented by the wave function $\psi(\mathbf{r}, t)e^{if(\mathbf{r}, t)/\hbar}$ provided we also change (in what is classically a harmless manner) the potentials to $V(\mathbf{r}, t) - \partial f(\mathbf{r}, t)/\partial t$ and $\mathbf{A}(\mathbf{r}, t) + \nabla f(\mathbf{r}, t)$ respectively. As noted in section (9.1), the new wave function still satisfies the usual Schrödinger equation formulated using the new potentials.

In the present interpretation of quantum mechanics we must view the matter differently. For, in the present interpretation, as we have seen, a change in potentials must certainly alter the motion of the particle so we cannot claim the evolving state of the particle is unchanged by a gauge transformation. Instead we claim that gauge invariance (in which we restrict the function f to satisfy $\nabla^2 f = 0$ in order to preserve the property $\nabla \cdot \mathbf{A} = 0$) reflects a correspondence between different (but *observationally equivalent*) states of knowledge under different potentials. Thus if G and G' are states of general knowledge differing with regard only to the potentials present, with G claiming the potentials are $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$, and G' claiming they are $V(\mathbf{r}, t) - \partial f(\mathbf{r}, t)/\partial t$ and $\mathbf{A}(\mathbf{r}, t) + \nabla f(\mathbf{r}, t)$, then for any pure state of knowledge Y of particle motion under G there is another pure state of knowledge Y' of particle motion under G' observationally equivalent to Y under G . If in the first case our wave function is $\psi(\mathbf{r}, t)$ and in the second $\psi'(\mathbf{r}, t)$ then these wave functions are related by $\psi'(\mathbf{r}, t) = \psi(\mathbf{r}, t)e^{if(\mathbf{r}, t)/\hbar}$. But under YG and under $Y'G'$ the expected frequencies of the results of any measurement of a kinematic property of the particle motion are equal in the two cases.*

* It is evident that the expected frequency for finding the particle in $d^3\mathbf{r}$ at time t is the same in the two cases since $|\psi'(\mathbf{r}, t)|^2 = |\psi(\mathbf{r}, t)|^2$. The corresponding particle momentum wave functions are not related in the same way, i.e. $|a'(\mathbf{p}, t)|^2 \neq |a(\mathbf{p}, t)|^2$, but this has to do with the fact that \mathbf{p} includes a contribution from the vector potential which is different in each case. Under gauge invariance (both in conventional quantum mechanics and in the present interpretation) constancy of expected frequencies

For a system of N distinguishable particles the general gauge transformation is given by

$$\left. \begin{aligned} \mathbf{A}_i &\rightarrow \mathbf{A}'_i = \mathbf{A}_i + \nabla_i f \\ V &\rightarrow V' = V - \frac{\partial f}{\partial t} \\ \psi &\rightarrow \psi' = \psi e^{\frac{i}{\hbar} f} \end{aligned} \right\} \quad (10.1)$$

where V, \mathbf{A}_i, ψ (and their primed versions) and f are generally all functions of the particle coordinates $\mathbf{r}_1, \dots, \mathbf{r}_N$ and the time t . To preserve the condition $\nabla \cdot \mathbf{A}_i = 0$ for $i = 1, \dots, N$ we restrict f to functions satisfying $\nabla_i^2 f = 0$ for $i = 1, \dots, N$. Under the transformation (10.1) the expected frequencies of the possible results of a measurement of any property of the motion (not involving the potentials) are preserved. That is ψ under V, \mathbf{A}_i and ψ' under V', \mathbf{A}'_i represent observationally equivalent states of knowledge. When ψ satisfies the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 \psi + V\psi + \sum_{i=1}^N \left(\frac{i\hbar}{m_i} \mathbf{A}_i \cdot \nabla_i \psi + \frac{A_i^2}{2m_i} \psi \right) \quad (10.2)$$

the transformation (10.1) results in ψ' satisfying the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi'}{\partial t} = -\sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 \psi' + V'\psi' + \sum_{i=1}^N \left(\frac{i\hbar}{m_i} \mathbf{A}'_i \cdot \nabla_i \psi' + \frac{A_i'^2}{2m_i} \psi' \right) \quad (10.3)$$

For completion we give the proof.

First note that by the last of (10.1)

$$\nabla_i \psi' = \left(\nabla_i \psi + \frac{i}{\hbar} \psi \nabla_i f \right) e^{\frac{i}{\hbar} f}$$

and that therefore

$$\nabla_i^2 \psi' = \left(\nabla_i^2 \psi + 2 \frac{i}{\hbar} \nabla_i f \cdot \nabla_i \psi - \frac{1}{\hbar^2} \psi (\nabla_i f)^2 \right) e^{\frac{i}{\hbar} f}.$$

Also

applies only to kinematic properties (like particle position and quantum mechanical particle velocity) which are not (gauge dependent) functions of the assumed potentials.

$$-\frac{\hbar}{i} \frac{\partial \psi'}{\partial t} = \left(-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} - \psi \frac{\partial f}{\partial t} \right) e^{\frac{i}{\hbar} f}.$$

Using these results we easily show, by substitution in (10.3), that (10.3) results in (10.2) and therefore that ψ' satisfies (10.3).

CHAPTER VII

SPIN ONE-HALF

1. Nature of spin in general

Spin is an internal dynamical property of a particle characterised by a dimensionless spin value s taking possible values $0, \frac{1}{2}, 1, \frac{3}{2}, \dots$. A system of particles (including a single particle system) may be known to have a net spin s (equal to one of the possible values $0, \frac{1}{2}, 1, \frac{3}{2}, \dots$) and a net magnetic moment μ both constant over a certain time period under prescribed conditions or both constant for all time in the case of a single particle whatever the conditions. It is then a 'spin s system'.

A spin s system has a dimensionless (generally time dependent) 'z component of spin' σ relative to a fixed Cartesian coordinate reference frame. At any one time and in any one such frame, σ has one of the discrete values $s, s-1, \dots -s$ (e.g. $\frac{1}{2}$ or $-\frac{1}{2}$ in the case $s = \frac{1}{2}$) representing a property of the system in that frame. A definite z component of spin (e.g. $\sigma = \frac{1}{2}$) in each coordinate system of different orientation (or of the same orientation occupied another way - see section 3.9 of Chapter III) represents a different property. But the same z components of spin in fixed coordinate systems that differ only by a simple *translation* in space, represent the *same* property.

All propositions concerning the z components of spin in fixed Cartesian coordinate systems over a time period constitute a complete sample space S_σ . The $2s+1$ propositions claiming one or other value of the z component of spin σ relative to a particular fixed Cartesian coordinate system at a certain time constitute a basis in S_σ , the natural order of this propositional basis being always given by the following order of the σ values claimed,

$$\sigma = s, s-1, \dots -s, \quad (1.1)$$

for example

$$\sigma = \frac{1}{2}, -\frac{1}{2}. \quad (1.2)$$

in the case $s = \frac{1}{2}$. Wave functions for spin using such a basis are normalised (complex valued) probability distributions $\psi(\sigma)$ over the possible values of σ .

A *particle* with spin s always has a (constant) magnetic moment. And, if an external magnetic field is present (possibly non-uniform and time-dependent), its spinning motion is dependent on the magnetic moment and on the magnetic field at the point occupied by the particle. That is, in any one fixed Cartesian coordinate frame whether or not the value of σ jumps to another value at any one time is dependent on the

size of the magnetic moment, and on the strength and direction of the magnetic field at the point occupied by the particle at that time and at times before.* If the particle carries a charge there may be an effect (on particle orbital motion) of the electromagnetic potential A_{em} associated with the magnetic field. But the magnetic field itself has no physical effect on the particle's orbital motion.† Despite this, propositions concerning the spinning motion and propositions concerning the orbital motion are only *logically* independent in the case of a *uniform* magnetic field. In a non-uniform magnetic field our knowledge of the particle position in space may clearly be of relevance with regard to our knowledge of its spinning motion and vice versa. Accordingly the sample space S_σ and the sample space S_r (of all propositions concerning the particle's position and momentum over the same time as that covered by S_σ) cannot (in general) be logically independent, and by the law of absolute logical independence (section 3.7 of Chapter I) we cannot generally hold pure knowledge $Y^{(1)}$ in S_σ and pure knowledge $Y^{(2)}$ in S_r . Therefore S_σ and S_r are not generally closed sample spaces. But the combined sample space $S_r S_\sigma$ is closed.

A system of particles known initially to have a spin s may not remain a spin s system when it experiences a magnetic field. This is because the magnetic field will generally act differently on the spin components of the individual particles which may have different magnetic moments or be in different parts of a non-uniform magnetic field. But since the z components of spin of all particles are amenable to the principle of short time isolation, a system of spin s will maintain its spin s for a short time after a magnetic field is switched on. And in certain circumstances (e.g. in a uniform magnetic field with certain relations holding between the magnetic moments of the particles making up the system) the system may remain indefinitely a spin s system carrying a constant (net) magnetic moment.

In the rest of this chapter we consider systems of particles (including single particle systems) having the particular spin value $s = \frac{1}{2}$.

2. Kinematic properties of the z components of spin one-half

With regard to a system of spin one-half, let the z component of spin relative to a fixed Cartesian coordinate system O be σ and let the z component of spin relative to another fixed Cartesian coordinate system O' sharing its origin with O be σ' . (Of course $s (= \frac{1}{2})$ is itself independent of the coordinate system.)

We will specify the state of O' relative to O using Euler angles α, β and γ , which denote (as in p 6-13 of [7]) a sequence of rotations of O that would get us to O' (i.e. that would put O into the same state as O'); we rotate O through angle β about the z axis of O , then through angle α about the new (temporary) x axis, then through

* As we consider only non-relativistic theory, we assume there is no particle spin/orbit interaction – this process can only be properly treated in a relativistic theory.

† This follows from the first law of potential action (section 3.2 of Chapter III) according to which a particle's orbital motion is not affected by the first spatial derivatives of the local vector potential.

angle γ about the new z axis; (all rotations being measured in the positive (right-handed) sense). Now α, β and γ may take any real values. But adding 4π to any one will of course change neither the orientation or the way O' occupies that orientation. Adding 2π to any one will not change the orientation but *will* change the way O' occupies that orientation.

Now, with regard to a system known to be a system of spin one-half with (constant) magnetic moment μ over a period of time, we claim the following kinematic properties of the z components of spin in O and O' during the time period.

First property The nature of the system carrying the spin $s = \frac{1}{2}$ and the magnetic moment μ has no bearing on the values of its z components of spin in O and O' (or in any fixed coordinate system) over the time period.

Second property If O and O' occupy the same orientation in the same way, then at any time t , a value of σ in O and an equal value of σ' in O' denote the same physical property.

Third property If the z axes of O and O' point in the same direction (i.e. if $\alpha = \gamma = 0$) then, whatever the value of β , a spin component σ in O at time t implies a spin component $\sigma' = \sigma$ in O' at time t . But it does so with a phase of implication equal to zero only when $\beta = 4\pi n$ (n any integer), i.e. only when O and O' occupy the same orientation in the same way.

Fourth property If the x axes of O and O' point in the same direction (i.e. if $\beta = \gamma = 0$) then at any one time, (i) a spin component σ in O implies (with zero phase of implication) a spin component $\sigma' = \sigma$ in O' only when $\alpha = 4\pi n$ (n any integer) and (ii) when $\alpha = \pm\pi$, a spin component σ in O implies a spin component $\sigma' = -\sigma$ in O' .

Fifth property If $\beta = 0$, $\alpha = -\pi$ and $\gamma = -\pi$ (or equivalently if coordinates O' are formed by rotating coordinates O through an angle $-\pi$ about the y axis*) then ' $\sigma = \frac{1}{2}$ in O at time t ' and ' $\sigma' = -\frac{1}{2}$ in O' at time t ' are fully equivalent propositions.

3. Spin/spin transformation functions

We seek the transformation functions $\Phi(\sigma|\sigma')$ and $\Phi(\sigma'|\sigma)$, the first being the probability distribution over the possible values of σ in O at time t knowing the value

* The band test (section 3.9 of Chapter III) shows this rotation to be exactly equivalent

of σ' in O' at time t and the second the probability distribution over the possible values of σ' in O' at time t knowing the value of σ in O at time t . Letting

$$\Phi(\sigma|\sigma') = \phi_{\sigma'}(\sigma), \quad (3.1)$$

$$\Phi(\sigma'|\sigma) = \phi_{\sigma}(\sigma') \quad (3.2)$$

where, for brevity, the same symbol ϕ is used to denote different (parameterised) functions $\phi_{\sigma}(\sigma)$ and $\phi_{\sigma}(\sigma')$, we have the necessary relations (see section 3.4 of Chapter I)

$$\phi_{\sigma}(\sigma') = (\phi_{\sigma'}(\sigma))^*, \quad (3.3)$$

$$\det[\Phi(\sigma|\sigma')] = \det[\Phi(\sigma'|\sigma)] = 1, \quad (3.4)$$

where, in the matrix equation (3.4), the matrix elements are labelled by the σ and σ' values in their natural order as in (1.2).*

The transformation functions $\phi_{\sigma'}(\sigma)$ are, by the first property in section 2, independent of the nature of the system of spin one-half and they are independent of any magnetic field that might be present.† The $\phi_{\sigma}(\sigma)$ are also the same (continuous and differentiable) functions of α, β and γ regardless of the time or of the orientation or position in space of the coordinate systems O and O' taken together as a pair. This follows from the isotropy of space and the homogeneity of space and time, for under any translation or rotation of coordinates O and O' taken together as a pair and for any change in the time $\phi_{\sigma}(\sigma)$ can, by the similarity principle, evidently change only by a phase factor $e^{i\delta}$ independent of σ and σ' , and of α, β and γ , but possibly dependent on the rotation and translation applied to O and O' and the change in time. But with $(\alpha, \beta, \gamma) = (0, 0, 0)$ we have, by the second property in section 2, $\phi_{\sigma}(\sigma) = \delta_{\sigma\sigma}$ both before and after the rotation or translation applied to O and O' , and the change in time, so $e^{i\delta}$ can only be equal to 1 and there can in fact be no change at all in the function $\phi_{\sigma}(\sigma)$. So $\phi_{\sigma}(\sigma)$ and $\phi_{\sigma}(\sigma')$ are universal functions of α, β and γ .

In matrix form we write (as in chapter 6 of [7]),

$$\phi_{\sigma}(\sigma') = \Phi(\sigma'|\sigma) = \begin{pmatrix} \Phi(\frac{1}{2}|\frac{1}{2}) & \Phi(\frac{1}{2}|\frac{-1}{2}) \\ \Phi(\frac{-1}{2}|\frac{1}{2}) & \Phi(\frac{-1}{2}|\frac{-1}{2}) \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \quad (3.5)$$

* So for example $\Phi(\frac{1}{2}|\frac{-1}{2})$ is the top right element of the 2×2 matrix $\Phi(\sigma|\sigma')$.

† This is because σ' represents a pure state of knowledge so that knowledge of the past history of the magnetic field is redundant. Knowledge of the future magnetic field is redundant because it has no effect on σ . And knowledge of the present magnetic field is redundant because σ is a property amenable to the principle of short time isolation.

a, b, c and d being functions of α, β and γ . Accordingly, Feynman's law connecting wave functions $\psi(\sigma)$ and $\psi'(\sigma')$ in O and O' can be written

$$\begin{pmatrix} \psi'(\frac{1}{2}) \\ \psi'(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} \psi(\frac{1}{2}) \\ \psi(-\frac{1}{2}) \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \psi(\frac{1}{2}) \\ \psi(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix} \begin{pmatrix} \psi'(\frac{1}{2}) \\ \psi'(-\frac{1}{2}) \end{pmatrix} \quad (3.6)$$

where, by the second property of section 2 and the second uniqueness property of probability assignment (section 5 of Chapter I),

$$a|_0 = d|_0 = 1, \quad b|_0 = c|_0 = 0 \quad (3.7)$$

subscripts zero denoting values at $(\alpha, \beta, \gamma) = (0, 0, 0)$.

4. Derivation of the transformation functions in the case of parallel z axes

Following the method employed by Feynman et al (see chapter 6 of [7]), we first derive the general form of $\phi_\sigma(\sigma')$ in the case O' could be realised by rotating O about the z axis through an angle β where $0 \leq \beta < 4\pi$.

By the third property of spin in section 2 we have

$$\phi_\sigma(\sigma') = \delta_{\sigma'\sigma} e^{ig(\sigma, \beta)} \quad (4.1)$$

where $g(\sigma, \beta)$ is a real function of σ and β continuous and differentiable in β and

$$g(\sigma, \beta) = 0 \pmod{2\pi} \quad \text{only for} \quad \beta = 4\pi n \quad (4.2)$$

where n is any integer.

We have seen that $\phi_\sigma(\sigma')$ and therefore $g(\sigma, \beta)$ depends only on the relative orientation of O and O' . Consider three coordinate systems O, O' and O'' , where O' would be realised by rotation of O through angle β_1 and O'' would be realised by rotation of O' through the angle β_2 or equivalently by rotation of O through angle β (where $\beta = \beta_1 + \beta_2$). Feynman's law gives

$$\Phi(\sigma''|\sigma) = \sum_{\sigma'} \Phi(\sigma''|\sigma') \Phi(\sigma'|\sigma)$$

or

$$\phi_\sigma(\sigma'') = \sum_{\sigma'} \phi_{\sigma'}(\sigma'') \phi_{\sigma'}(\sigma)$$

or, by (4.1),

$$\delta_{\sigma'\sigma} e^{ig(\sigma, \beta_1 + \beta_2)} = \sum_{\sigma'} \delta_{\sigma'\sigma'} e^{ig(\sigma', \beta_2)} \cdot \delta_{\sigma'\sigma} e^{ig(\sigma, \beta_1)} = \delta_{\sigma'\sigma} e^{i(g(\sigma, \beta_1) + g(\sigma, \beta_2))}$$

implying that $g(\sigma, \beta)$ must satisfy

$$g(\sigma, \beta_1 + \beta_2) = g(\sigma, \beta_1) + g(\sigma, \beta_2)$$

or must be a homogeneous linear function of β :

$$g(\sigma, \beta) = g(\sigma)\beta. \quad (4.3)$$

Hence

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} e^{ig(\frac{1}{2})\beta} & 0 \\ 0 & e^{ig(-\frac{1}{2})\beta} \end{pmatrix}.$$

where the determinant condition (3.4) gives $g(\frac{1}{2}) + g(-\frac{1}{2}) = 0$ or $g(\frac{1}{2}) = -g(-\frac{1}{2}) = \lambda$ in which, by (4.2) and (4.3), λ can be only $\pm \frac{1}{2}$. Hence

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} e^{i\lambda\beta} & 0 \\ 0 & e^{-i\lambda\beta} \end{pmatrix}, \quad \lambda = \pm \frac{1}{2}. \quad (4.4)$$

(Later we will use the freedom to choose a wave function or its conjugate (section 8 of Chapter I) to set $\lambda = \frac{1}{2}$, but for the present we leave the choice of λ unspecified.)

5. Derivation of the transformation functions in the case of a general rotation

To obtain the transformation functions for a general rotation we first derive their form in the case of rotations about the x axis. Then using this result and the result in section 4 we derive the transformation functions for a general rotation by applying successive rotations about the (original) z axis, the (temporary new) x axis, and the (new) z axis.

Case of rotations about the x axis

Here only the Euler angle α is different from zero. A rotation of axes O by α about the x axis to give new axes O' followed by a infinitesimal rotation $d\alpha$ to give new axes O'' is equivalent to a single rotation $\alpha + d\alpha$ giving O'' directly from O . This implies the following matrix equation:

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} \Big|_{\alpha+d\alpha} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \Big|_{d\alpha} \begin{pmatrix} a & c \\ b & d \end{pmatrix} \Big|_{\alpha} \quad (5.1)$$

where the subscript denotes the value of α in the matrix elements a, b, c and d , and (below) in their first derivatives. Clearly

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} \Big|_{\alpha+d\alpha} = \begin{pmatrix} a + \frac{\partial a}{\partial \alpha} d\alpha & c + \frac{\partial c}{\partial \alpha} d\alpha \\ b + \frac{\partial b}{\partial \alpha} d\alpha & d + \frac{\partial d}{\partial \alpha} d\alpha \end{pmatrix} \Big|_{\alpha} \quad (5.2)$$

and by (3.7)

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} \Big|_{d\alpha} = \begin{pmatrix} 1 + \tilde{a}_0 d\alpha & \tilde{c}_0 d\alpha \\ \tilde{b}_0 d\alpha & 1 + \tilde{d}_0 d\alpha \end{pmatrix} \quad (5.3)$$

where

$$\tilde{a}_0 = \frac{\partial a}{\partial \alpha} \Big|_0, \quad \tilde{b}_0 = \frac{\partial b}{\partial \alpha} \Big|_0, \quad \tilde{c}_0 = \frac{\partial c}{\partial \alpha} \Big|_0, \quad \tilde{d}_0 = \frac{\partial d}{\partial \alpha} \Big|_0. \quad (5.4)$$

Substituting (5.2) and (5.3) into (5.1), multiplying out the matrix product on the RHS and equating matrix elements on the two sides gives

$$\left. \begin{aligned} \frac{\partial a}{\partial \alpha} &= \tilde{a}_0 a + \tilde{c}_0 b \\ \frac{\partial b}{\partial \alpha} &= \tilde{b}_0 a + \tilde{d}_0 b \\ \frac{\partial c}{\partial \alpha} &= \tilde{a}_0 c + \tilde{c}_0 d \\ \frac{\partial d}{\partial \alpha} &= \tilde{b}_0 c + \tilde{d}_0 d \end{aligned} \right\} \quad (5.5)$$

From the orthonormality of transformation functions we require

$$\left. \begin{aligned} a^* a + b^* b &= 1 \\ a^* c + b^* d &= 0 \\ c^* c + d^* d &= 1 \end{aligned} \right\}$$

Differentiating these with respect to α and setting α equal to zero gives

$$\left. \begin{aligned} \tilde{a}_0 &= i\alpha_0 \\ \tilde{c}_0 &= -\tilde{b}_0^* \\ \tilde{d}_0 &= i\delta_0 \end{aligned} \right\} \quad (5.6)$$

where α_0 and δ_0 are certain real numbers.

From the requirement for phase normalisation, i.e. by (3.4), we have

$$ad - bc = 1.$$

Differentiating this with respect to α and setting $\alpha = 0$ gives

$$\tilde{d}_0 = -\tilde{a}_0 \quad (5.7)$$

Differentiating each of (5.5) with respect to α and using (5.5) themselves to eliminate the first derivatives, we find with the help of (5.6) and (5.7) that

$$\frac{\partial^2 a}{\partial \alpha^2} = -k^2 a, \quad \frac{\partial^2 b}{\partial \alpha^2} = -k^2 b, \quad \frac{\partial^2 c}{\partial \alpha^2} = -k^2 c, \quad \frac{\partial^2 d}{\partial \alpha^2} = -k^2 d \quad (5.8)$$

where

$$k^2 = |\tilde{b}_0|^2 - \alpha_0^2. \quad (5.9)$$

It is evident that $k \neq 0$ for then (5.8) would make a, b, c, d linear functions of α which reduce to $a = d = 1, c = b = 0$ on account of the 'boundary conditions' at $\alpha = 0, 4\pi$. And this would contradict the fourth property of spin.

Solving the differential equations (5.8) we have

$$\left. \begin{aligned} a &= A_1 e^{ik\alpha} + A_2 e^{-ik\alpha} \\ b &= B_1 e^{ik\alpha} + B_2 e^{-ik\alpha} \\ c &= C_1 e^{ik\alpha} + C_2 e^{-ik\alpha} \\ d &= D_1 e^{ik\alpha} + D_2 e^{-ik\alpha} \end{aligned} \right\} \quad (5.10)$$

where the constant coefficients can be found from the 'boundary conditions' on a, b, c, d and their first derivatives at $\alpha = 0$. The result is

$$\left. \begin{aligned} a &= \cos k\alpha + i \frac{\alpha_0}{k} \sin k\alpha \\ b &= \frac{\tilde{b}_0}{k} \sin k\alpha \\ c &= -\frac{\tilde{b}_0^*}{k} \sin k\alpha \\ d &= \cos k\alpha - i \frac{\alpha_0}{k} \sin k\alpha \end{aligned} \right\} \quad (5.11)$$

For $\alpha \rightarrow \alpha + 4\pi$ we know the transformation functions must return to the same form, i.e. $a(\alpha + 4\pi) = a(\alpha)$, $b(\alpha + 4\pi) = b(\alpha)$, ... etc. By (5.11) this means $\cos k\alpha$ and $\sin k\alpha$ (and therefore $e^{ik\alpha}$) are periodic functions of α with period 4π . Therefore $e^{ik4\pi} = e^{ik0} = 1$ and k must have one of the half-integer values

$$k = \pm \frac{1}{2}, \pm 1, \pm \frac{3}{2}, \dots \quad (5.12)$$

Now we apply part (ii) of the fourth property of spin in section 2 to obtain

$$\left(\begin{array}{cc} a & c \\ b & d \end{array} \right) \Big|_{\alpha=\pi} = \left(\begin{array}{cc} 0 & e^{i\mu} \\ e^{i\eta} & 0 \end{array} \right)$$

where μ and η are real constants. This gives, from (5.11),

$$\left. \begin{aligned} \cos k\pi &= -i \frac{\alpha_0}{k} \sin k\pi = i \frac{\alpha_0}{k} \sin k\pi \\ \frac{\tilde{b}_0}{k} \sin k\pi &= e^{i\eta} \end{aligned} \right\}$$

The first shows that α_0 can only be zero and that k is limited to half-odd-integer values. And as a result the second shows that

$$\frac{\tilde{b}_0}{k} = e^{i\phi} \quad (5.13)$$

for some real function ϕ of k (i.e. of its half-odd-integer value).

To see which half-odd-integer value of k applies consider the probability for $\sigma' = \frac{1}{2}$ in O' when we know $\sigma = \frac{1}{2}$ in O . By (3.5) this is

$$\Phi\left(\frac{1}{2} \Big| \frac{1}{2}\right) = a = \cos k\alpha$$

since $\alpha_0 = 0$ in the first of (5.11). But by part (i) of the fourth property of spin $\Phi\left(\frac{1}{2} \middle| \frac{1}{2}\right)$ is equal to 1 only for $\alpha = 4\pi n$ (n any integer) therefore k can only be equal to $\pm \frac{1}{2}$.

We thus reach the following form for the transformation matrix in the case of rotations through any angle α about the x axis:

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} \cos \frac{\alpha}{2} & -e^{-i\phi} \sin \frac{\alpha}{2} \\ e^{i\phi} \sin \frac{\alpha}{2} & \cos \frac{\alpha}{2} \end{pmatrix}. \quad (5.14)$$

We establish the value of the remaining real constant ϕ by considering general rotations and applying the fifth property of spin.

Case of general rotations

Under any rotation of O through successive Euler angles β, α, γ we clearly have by (4.4) and (5.14), that the form of the general transformation matrix in (3.5) is given by the following product:

$$\begin{aligned} \begin{pmatrix} a & c \\ b & d \end{pmatrix} &= \begin{pmatrix} e^{i\lambda\gamma} & 0 \\ 0 & e^{-i\lambda\gamma} \end{pmatrix} \begin{pmatrix} \cos \frac{\alpha}{2} & -e^{-i\phi} \sin \frac{\alpha}{2} \\ e^{i\phi} \sin \frac{\alpha}{2} & \cos \frac{\alpha}{2} \end{pmatrix} \begin{pmatrix} e^{i\lambda\beta} & 0 \\ 0 & e^{-i\lambda\beta} \end{pmatrix} \\ &= \begin{pmatrix} \cos \frac{\alpha}{2} e^{i\lambda(\beta+\gamma)} & -e^{-i\phi} \sin \frac{\alpha}{2} e^{-i\lambda(\beta-\gamma)} \\ e^{i\phi} \sin \frac{\alpha}{2} e^{i\lambda(\beta-\gamma)} & \cos \frac{\alpha}{2} e^{-i\lambda(\beta+\gamma)} \end{pmatrix} \end{aligned} \quad (5.15)$$

To fix the value of $e^{i\phi}$ we apply the fifth property of spin in section 2. By the first of (3.6) the fifth property of spin tells us that

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} \Big|_{\substack{\beta=0 \\ \alpha=-\pi \\ \gamma=-\pi}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

which gives $b \Big|_{\substack{\beta=0 \\ \alpha=-\pi \\ \gamma=-\pi}} = 1$, or, by (5.15), $-e^{i\phi} e^{i\lambda\pi} = 1$, Therefore $e^{i\phi} = \pm i$ according as

$\lambda = \pm \frac{1}{2}$. Substituting these alternatives into (5.15) gives a certain matrix or its conjugate according as we take $\lambda = \frac{1}{2}$ or $\lambda = -\frac{1}{2}$. Since we have not yet established the absolute form (one form or its conjugate) of any wave function to do with spin one-half, we are at liberty to choose which value of λ to take. In agreement with the normal convention we choose to make $\lambda = \frac{1}{2}$ and hence establish the spin/spin transformation matrix as

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} \cos \frac{\alpha}{2} e^{i(\beta+\gamma)/2} & i \sin \frac{\alpha}{2} e^{-i(\beta-\gamma)/2} \\ i \sin \frac{\alpha}{2} e^{i(\beta-\gamma)/2} & \cos \frac{\alpha}{2} e^{-i(\beta+\gamma)/2} \end{pmatrix} \quad (5.16)$$

The transformation functions $\phi_\sigma(\sigma')$ are of course expressed in terms of the matrix elements by (3.5) now given explicitly by (5.16), and the transformation function $\phi_\sigma(\sigma)$, which is just the conjugate of $\phi_\sigma(\sigma')$ is, in matrix form, the conjugate of the transpose of the matrix on the RHS of (5.16) as in (3.6).

6. Wave function for spin with a known component in a given direction

Let O and O' be fixed coordinate systems sharing an origin. Let O' be obtained by rotating O through Euler angles $\beta = \phi + \frac{\pi}{2}$, $\alpha = \theta$ and γ equal to any given angle. The z' direction is then specified (in O) by spherical polar angles θ and ϕ , θ being the angle between the z axis and the z' direction, and ϕ the angle between the x axis and the projection of the z' direction onto the xy plane.

If we know $\sigma' = \frac{1}{2}$ in O' then in O our wave function $\psi(\sigma) = \Phi(\sigma|_{\frac{1}{2}}')$ is (by (3.6))

$$\begin{pmatrix} \psi(\frac{1}{2}) \\ \psi(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a^* \\ c^* \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \sin \frac{\theta}{2} e^{i\frac{\phi}{2}} \end{pmatrix} e^{-i\frac{1}{2}(\gamma + \frac{\pi}{2})}. \quad (6.1)$$

Evidently, for various specified values of γ , or for unspecified γ , our states of knowledge of the physical world are the same as regards the spinning motion itself (see section 3.3 of Chapter I). In the case of unspecified γ (i.e. given only the spin component in a direction specified by polar angles θ and ϕ) our wave function is accordingly

$$\begin{pmatrix} \psi(\frac{1}{2}) \\ \psi(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \sin \frac{\theta}{2} e^{i\frac{\phi}{2}} \end{pmatrix} e^{i\lambda}. \quad (6.2)$$

where $\lambda (= -\frac{1}{2}(\gamma + \frac{\pi}{2}))$ is an unspecified constant phase. If the means of recovering knowledge of γ (which must have been initially given when acquiring the knowledge $\sigma' = \frac{1}{2}$ in O') is irretrievably lost then λ is an *indeterminate* phase.

Knowledge that $\sigma' = \frac{1}{2}$ in O' at time t , with given θ and ϕ , and with specified unspecified, partially specified or indeterminate γ , is the general pure state of knowledge in relation to the sample space S_σ . The corresponding wave functions ((6.1) and (6.2)) cover all the possible wave functions in O at time t and these are in fact all the possible normalised 2-D column vectors of complex-valued components with determinate relative

phases and determinate, unspecified, partially specified or indeterminate absolute phases.*

Alternatively, if we know $\sigma' = -\frac{1}{2}$ in O' then, in O our wave function $\psi(\sigma)$ is

$$\begin{pmatrix} \psi(\frac{1}{2}) \\ \psi(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} -\sin \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \cos \frac{\theta}{2} e^{i\frac{\phi}{2}} \end{pmatrix} e^{i\frac{1}{2}(\gamma+\pi)} \quad (6.3)$$

in place of (6.1), and our wave function given only that the spin component is $-\frac{1}{2}$ in a direction specified by polar angles θ and ϕ is

$$\begin{pmatrix} \psi(\frac{1}{2}) \\ \psi(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} -\sin \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \cos \frac{\theta}{2} e^{i\frac{\phi}{2}} \end{pmatrix} e^{-i\lambda} \quad (6.4)$$

where λ is here the same constant λ as in (6.2).

7. The x and y components of spin

In the usual formalism of quantum mechanics we have, relative to any one fixed Cartesian coordinate system O , components of spin σ_x in the x direction and σ_y in the y direction (as well as the component σ in the z direction). The wave functions in σ for known values ($+\frac{1}{2}$ or $-\frac{1}{2}$) of σ_x or for known values ($+\frac{1}{2}$ or $-\frac{1}{2}$) of σ_y are represented by eigenvectors of the operators $\hat{\sigma}_x$ and $\hat{\sigma}_y$ respectively where

$$\hat{\sigma}_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (7.1)$$

In the case of $\hat{\sigma}_x$ these eigenvectors are

* Any coordinate system O' sharing its origin with O is represented uniquely by (θ, ϕ, γ) with $0 \leq \theta \leq \pi$, $0 \leq \phi < 2\pi$ and $0 \leq \gamma < 4\pi$. With the same ranges for θ, ϕ and γ , any normalised 2-D column vector $\{Ae^{i\alpha}, Be^{i\beta}\}$ ($A^2 + B^2 = 1$) is represented uniquely by the RHS of (6.1). For θ fixed $\cos \frac{\theta}{2}$ and $\sin \frac{\theta}{2}$ (i.e. A and B) uniquely, and thinking of α and β as points on the unit circle in the complex plane represented by their angular position (their arguments) α and β with $\beta - \alpha$ positive or zero, the relative position of β with respect to α is fixed by ϕ ($= \beta - \alpha$) and finally the absolute position of α is fixed by γ in the relation $\alpha = -\frac{\phi}{2} - \frac{\gamma}{2} - \frac{\pi}{4}$.

$$\Phi(\sigma|\sigma_x = \frac{1}{2}) = \begin{pmatrix} \frac{1}{\sqrt{2}} e^{i\delta} \\ \frac{1}{\sqrt{2}} e^{i\delta} \end{pmatrix}, \quad \Phi(\sigma|\sigma_x = -\frac{1}{2}) = \begin{pmatrix} \frac{1}{\sqrt{2}} e^{i\varepsilon} \\ -\frac{1}{\sqrt{2}} e^{i\varepsilon} \end{pmatrix} \quad (7.2)$$

with eigenvalues $\sigma_x = \frac{1}{2}, -\frac{1}{2}$ respectively. They are determined only to within arbitrary phase factors $e^{i\delta}$ and $e^{i\varepsilon}$.

In the present interpretation of quantum mechanics we identify the properties of the x and y components of spin in O (for spin of any magnitude, not just for $s = \frac{1}{2}$) with the z components of spin in coordinates O' formed by rotating coordinates O through the Euler angles $(\alpha, \beta, \gamma) = (-\pi/2, -\pi/2, \pi/2)$ and $(\alpha, \beta, \gamma) = (-\pi/2, 0, 0)$ respectively, or equivalently by rotating O by $+\pi/2$ about the y axis and $-\pi/2$ about the x axis respectively. It follows that the properties of the x and y components of spin in O are each basic properties and we obtain (for $s = \frac{1}{2}$), in the case of σ_x the transformation functions

$$\Phi(\sigma|\sigma_x) = \Phi(\sigma|\sigma') = \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix}_{\substack{\alpha=-\pi/2 \\ \beta=-\pi/2 \\ \gamma=\pi/2}} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (7.3)$$

derived from (5.16). These agree with (7.2) with $\delta = 0$ and $\varepsilon = \pi$. Similarly in the case of σ_y we obtain the transformation functions

$$\Phi(\sigma|\sigma_y) = \Phi(\sigma|\sigma') = \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix}_{\substack{\alpha=-\pi/2 \\ \beta=\gamma=0}} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}i \\ \frac{1}{\sqrt{2}}i & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (7.4)$$

the two columns in the matrix being eigenvectors of $\hat{\sigma}_y$ in (7.1). On account of us identifying the x and y components of spin in the way we have, the transformation functions $\Phi(\sigma|\sigma_x)$ and $\Phi(\sigma|\sigma_y)$ have definite absolute phases.

The basic properties σ_x and σ_y have operators $\hat{\sigma}_x$ and $\hat{\sigma}_y$ associated with them as all basic properties do (see section 6.2 of Chapter II). We can derive the form of these operators (as quoted in matrix form in (7.1)) from the defining rules

$$\hat{\sigma}_x \Phi(\sigma|\sigma_x) = \sigma_x \Phi(\sigma|\sigma_x), \quad (7.5)$$

$$\hat{\sigma}_y \Phi(\sigma|\sigma_y) = \sigma_y \Phi(\sigma|\sigma_y), \quad (7.6)$$

(c.f. (6.2.1) of Chapter II). The first has to hold for all values of σ_x (i.e. for $\sigma_x = \frac{1}{2}$ and $\sigma_x = -\frac{1}{2}$) and the second for all values of σ_y (for $\sigma_y = \frac{1}{2}$ and $\sigma_y = -\frac{1}{2}$).

To obtain the matrix expression for $\hat{\sigma}_x$ we write

$$\hat{\sigma}_x = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

where α, β, γ and δ are complex constants to be determined and we rewrite (7.5) as

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} \Phi(\frac{1}{2}|\sigma_x) \\ \Phi(-\frac{1}{2}|\sigma_x) \end{pmatrix} = \sigma_x \begin{pmatrix} \Phi(\frac{1}{2}|\sigma_x) \\ \Phi(-\frac{1}{2}|\sigma_x) \end{pmatrix} \quad (7.7)$$

holding for $\sigma_x = \frac{1}{2}$ and $\sigma_x = -\frac{1}{2}$. The two relations (7.7) (one for each value of σ_x) can be written together as the single relation

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} \Phi(\frac{1}{2}|\frac{1}{2}) & \Phi(\frac{1}{2}|-\frac{1}{2}) \\ \Phi(-\frac{1}{2}|\frac{1}{2}) & \Phi(-\frac{1}{2}|-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\Phi(\frac{1}{2}|\frac{1}{2}) & -\frac{1}{2}\Phi(\frac{1}{2}|-\frac{1}{2}) \\ \frac{1}{2}\Phi(-\frac{1}{2}|\frac{1}{2}) & -\frac{1}{2}\Phi(-\frac{1}{2}|-\frac{1}{2}) \end{pmatrix} \quad (7.8)$$

Here the second matrix on the LHS is just the matrix $[\Phi(\sigma|\sigma_x)]$ in the notation used in the ‘law of unit determinant’ (section 3.4 of Chapter I). By the law of orthogonality of transformation functions ((3.4.3) of Chapter I) we have, in matrix notation

$$[\Phi(\sigma|\sigma_x)][\Phi^*(\sigma_x|\sigma)] = [1]$$

where [1] is the unit 2×2 matrix. Therefore $[\Phi^*(\sigma_x|\sigma)]$ is the inverse of matrix $[\Phi(\sigma|\sigma_x)]$, and it is given by the transpose of the conjugate of the matrix in (7.3). i.e. by

$$[\Phi^*(\sigma_x|\sigma)] = \begin{pmatrix} a & c \\ b & d \end{pmatrix}_{\substack{\alpha=-\pi/2 \\ \beta=-\pi/2 \\ \gamma=\pi/2}} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}. \quad (7.9)$$

The matrix on the RHS of (7.8) is, by (7.3),

$$\begin{pmatrix} \frac{1}{2}\frac{1}{\sqrt{2}} & (-\frac{1}{2})(-\frac{1}{\sqrt{2}}) \\ \frac{1}{2}\frac{1}{\sqrt{2}} & (-\frac{1}{2})\frac{1}{\sqrt{2}} \end{pmatrix}.$$

Substituting this on the RHS of (7.8) and multiplying each side of (7.8) on the right by the matrix (7.9) we obtain

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\frac{1}{\sqrt{2}} & (-\frac{1}{2})(-\frac{1}{\sqrt{2}}) \\ \frac{1}{2}\frac{1}{\sqrt{2}} & (-\frac{1}{2})\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

which is the same as $\hat{\sigma}_x$ in the first of (7.1).

Similarly we can establish from (7.6) the form for $\hat{\sigma}_y$ quoted in the second of (7.1).

And of course we can formally introduce the operator $\hat{\sigma}_z$ going with the z component of spin σ_z (so far denoted σ). This is defined by the relation

$$\hat{\sigma}_z \Phi(\sigma|\sigma_z) = \sigma_z \Phi(\sigma|\sigma_z) \quad (7.10)$$

for $\sigma_z = \frac{1}{2}$ and $\sigma_z = -\frac{1}{2}$. Since $\Phi(\sigma|\sigma_z) = \delta_{\sigma\sigma_z}$, this relation in matrix form is

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \cdot 1 & -\frac{1}{2} \cdot 0 \\ \frac{1}{2} \cdot 0 & -\frac{1}{2} \cdot 1 \end{pmatrix}$$

where the first matrix on the LHS now represents $\hat{\sigma}_z$. Therefore $\hat{\sigma}_z$ in matrix form is

$$\sigma_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (7.11)$$

8. Spinning motion in a uniform magnetic field

A spin one-half system has a constant magnetic moment μ associated with its spin, the dimensions of magnetic moment being those of energy divided by magnetic field intensity. Its spinning motion is therefore affected by a uniform external magnetic field of intensity $\mathbf{H}(t)$.^{*} That is, the way in which the z component of spin σ (relative to any one fixed coordinate system O) changes abruptly from time to time (between the values $\frac{1}{2}$ and $-\frac{1}{2}$) depends in some way on $\mathbf{H}(t)$ and on μ but not on the peculiar nature of the system carrying the spin one-half. We claim the following properties regarding the dependence of spin components on the field, the magnetic moment and the time.

First property During any short time t to $t + dt$ the value of σ in any fixed Cartesian coordinate system is affected by the momentary value $\mathbf{H}(t)$ of \mathbf{H} but not by the time derivative of $\mathbf{H}(t)$ or by higher

^{*} Although the magnetic field $\mathbf{H}(t)$ is always uniform in space, we allow its magnitude *and direction* to change in time.

time derivatives of $\mathbf{H}(t)$ at time t , or of course by the value of $\mathbf{H}(t)$ at times greater than $t + dt$.*

Second property Suppose, relative to fixed coordinates O , that $\mathbf{H}(t) = H\hat{\mathbf{k}}$, i.e. that the field is parallel to the z axis and constant in time. Then (i) σ in O is constant in time, and (ii) the z components of spin in all fixed coordinate systems are each periodic functions of the time with period $\pi\hbar/\mu H$ and they do not all return to their same values in any time less than $\pi\hbar/\mu H$.

8.1 Spin/spin transformation functions over time in a constant magnetic field.

Relative to a fixed Cartesian coordinate system O we denote by $\Phi(\sigma t|\sigma_1 t_1)$ the transformation function that will take us from any wave function over the z component of spin (denoted σ_1) in O at time t_1 to the corresponding wave function over σ in O at time t . Clearly $\Phi(\sigma t|\sigma_1 t_1)$ is independent of the position of the origin of the coordinates in space and of the nature of the system carrying the spin one-half.

Case of \mathbf{H} parallel to the z axis of coordinates

With $\mathbf{H} = H\hat{\mathbf{k}}$ ($H = \text{const.}$) part (i) of the second property of spinning motion in a magnetic field tells us that the transformation function $\Phi(\sigma t|\sigma_1 t_1)$ between spin component σ_1 at time t_1 and spin component σ at time t has the form

$$\Phi(\sigma t|\sigma_1 t_1) = \delta_{\sigma\sigma_1} e^{i\varepsilon(t-t_1, t_1, \sigma_1)} \quad (8.1.1)$$

where ε must be a real-valued differentiable function of $t - t_1$ and t_1 , and

$$\varepsilon(0, t_1, \sigma_1) = 0 \quad (8.1.2)$$

since at $t = t_1$ equal values of σ and σ_1 represent the same property.

If we shift the origin of the time by any amount δ , the problem of finding $\Phi'(\sigma t|\sigma_1 t_1) (= \delta_{\sigma\sigma_1} e^{i\varepsilon'(t-t_1, t_1, \sigma_1)})$ using the new time coordinate is (by the homogeneity of time) *similar* to the problem of finding $\Phi(\sigma t|\sigma_1 t_1) (= \delta_{\sigma\sigma_1} e^{i\varepsilon(t-t_1, t_1, \sigma_1)})$ in the original time coordinate. Therefore, by (5.1.2) of Chapter I we have the functional relation

$$\delta_{\sigma\sigma_1} e^{i\varepsilon'(t-t_1, t_1, \sigma_1)} = \delta_{\sigma\sigma_1} e^{i\varepsilon(t-t_1, t_1, \sigma_1)} e^{i\alpha}$$

* In the case of a *particle* of spin one-half, this property is generalised (in section 9.2) to cover also the lack of any effect of the spatial derivatives of a *non-uniform* magnetic field.

where the phase α is independent of σ, σ_1, t and t_1 . Also, by the uniqueness of probability assignment $\varepsilon'(t-t_1, t_1, \sigma_1) = \varepsilon(t-t_1, t_1 + \delta, \sigma_1) + \alpha$ where by (8.1.2) α must be zero, and accordingly $\varepsilon(t-t_1, t_1, \sigma_1)$ is independent of its second variable and can be replaced by $\varepsilon(t-t_1, \sigma_1)$. So we can change (8.1.1) to

$$\Phi(\sigma t | \sigma_1 t_1) = \delta_{\sigma\sigma_1} e^{i\varepsilon(t-t_1, \sigma_1)} \quad (8.1.3)$$

and (8.1.2) gives

$$\varepsilon(0, \sigma_1) = 0. \quad (8.1.4)$$

Because of the isotropy of space and the similarity principle $\Phi(\sigma t | \sigma_1 t_1)$ in (8.1.3) (and therefore $\varepsilon(t-t_1, \sigma_1)$) is a *universal* function of $t-t_1$ and σ_1 , i.e. one independent of any rotation of the coordinate system and magnetic field together. The constant phase factor that might be multiplying the wave function $\Phi(\sigma t | \sigma_1 t_1)$ after such a rotation must be independent of $t-t_1$, and on account of (8.1.4) it can only equal 1.

Introducing another time t_2 we now apply Feynman's law

$$\Phi(\sigma t | \sigma_1 t_1) = \sum_{\sigma_2} \Phi(\sigma t | \sigma_2 t_2) \Phi(\sigma_2 t_2 | \sigma_1 t_1).$$

Using (8.1.3) this gives

$$\delta_{\sigma\sigma_1} e^{i\varepsilon(t-t_1, \sigma_1)} = \sum_{\sigma_2} \delta_{\sigma\sigma_2} e^{i\varepsilon(t-t_2, \sigma_2)} \delta_{\sigma_2\sigma_1} e^{i\varepsilon(t_2-t_1, \sigma_1)} = \delta_{\sigma\sigma_1} e^{i(\varepsilon(t-t_2, \sigma_1) + \varepsilon(t_2-t_1, \sigma_1))}$$

implying

$$\varepsilon(t-t_1, \sigma_1) = \varepsilon(t-t_2, \sigma_1) + \varepsilon(t_2-t_1, \sigma_1).$$

As this must hold for any t , $\varepsilon(t, \sigma)$ must be a homogeneous linear function of t . Hence (8.1.3) becomes

$$\Phi(\sigma t | \sigma_1 t_1) = \delta_{\sigma\sigma_1} e^{i\varepsilon(\sigma_1)(t-t_1)}.$$

Now $\varepsilon(\sigma_1)$ can depend only on μ, H and the fundamental constant \hbar . So from dimensional considerations it must be that $\varepsilon(\sigma_1) = f(\sigma_1) \frac{\mu H}{\hbar}$ where $f(\sigma_1)$ is a real-valued universal dimensionless function of σ_1 . Hence $\Phi(\sigma t | \sigma_1 t_1) = \delta_{\sigma\sigma_1} e^{if(\sigma_1) \frac{\mu H}{\hbar} (t-t_1)}$ and applying the unit determinant condition:

$$\det[\Phi(\sigma t|\sigma_1 t_1)] = e^{if(\frac{1}{2})\frac{\mu H}{\hbar}(t-t_1)} \cdot e^{if(-\frac{1}{2})\frac{\mu H}{\hbar}(t-t_1)} = 1$$

we find $f(\frac{1}{2}) + f(-\frac{1}{2}) = 0$ or $f(\frac{1}{2}) = -f(-\frac{1}{2}) = k$, where k is a universal (real-valued) numerical constant. In matrix notation we therefore have

$$\Phi(\sigma t|\sigma_1 t_1) = \begin{pmatrix} e^{ik\frac{\mu H}{\hbar}(t-t_1)} & 0 \\ 0 & e^{-ik\frac{\mu H}{\hbar}(t-t_1)} \end{pmatrix}. \quad (8.1.5)$$

Now by part (ii) of the second property of spinning motion in a magnetic field, starting at time t_1 and assuming μH is positive, the z components of spin in all fixed coordinate systems return to their same values for the first time when $t = t_1 + \pi\hbar/\mu H$. Before this time at least some of the z components of spin are different from their initial values. This means that, in a fixed coordinate system O' formed by rotating O through Euler angles (α, β, γ) , σ' does not generally return to the value $\sigma'(t_1)$ it had at time t_1 till $t = t_1 + \pi\hbar/\mu H$. Certainly the σ' components for every orientation (α, β, γ) do not *all* return to their initial values *simultaneously* at any time between t_1 and $t = t_1 + \pi\hbar/\mu H$. Accordingly we cannot have

$$\Phi(\sigma' t|\sigma' t_1) = e^{i\phi(\alpha, \beta, \gamma)} \quad (8.1.6)$$

with $\phi(\alpha, \beta, \gamma)$ determinate for *all* (α, β, γ) at any one time t in the range $t_1 < t < t_1 + \pi\hbar/\mu H$, for this would mean that $\sigma' t_1 \Rightarrow^\phi \sigma' t$ with a determinate phase of implication for any (α, β, γ) , or that the z components of spin *do* all return to exactly the same values before time $t_1 + \pi\hbar/\mu H$.

Now applying Feynman's law twice we have for general spin components σ' and σ'_1 in O' that

$$\Phi(\sigma' t|\sigma'_1 t_1) = \sum_{\sigma} \sum_{\sigma_1} \Phi(\sigma' t|\sigma t) \Phi(\sigma t|\sigma_1 t_1) \Phi(\sigma_1 t_1|\sigma'_1 t_1)$$

where σ and σ_1 refer to O . In the matrix notation this is, by (3.6) and (8.1.5)

$$\Phi(\sigma' t|\sigma'_1 t_1) = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} e^{ik\varepsilon} & 0 \\ 0 & e^{-ik\varepsilon} \end{pmatrix} \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix}$$

where

$$\varepsilon = \frac{\mu H}{\hbar} (t - t_1) \quad (8.1.7)$$

Multiplying out the matrices and applying the result (5.16) we thus find

$$\Phi\left(\frac{1'}{2} t \middle| \frac{1'}{2} t_1\right) = aa^* e^{ik\varepsilon} + cc^* e^{-ik\varepsilon} = \cos^2 \frac{\alpha}{2} e^{ik\varepsilon} + \sin^2 \frac{\alpha}{2} e^{-ik\varepsilon} \quad (8.1.8)$$

$$\Phi\left(-\frac{1'}{2} t \middle| -\frac{1'}{2} t_1\right) = bb^* e^{ik\varepsilon} + dd^* e^{-ik\varepsilon} = \sin^2 \frac{\alpha}{2} e^{ik\varepsilon} + \cos^2 \frac{\alpha}{2} e^{-ik\varepsilon} \quad (8.1.9)$$

for the specific values $\sigma' = \sigma'_1 = +\frac{1}{2}$ and $-\frac{1}{2}$ respectively.

For (8.1.6) to hold, as it should for $t = t_1 + \pi\hbar/\mu H$ (or for $\varepsilon = \pi$), it must be that

$$\left| \Phi\left(\frac{1'}{2} t \middle| \frac{1'}{2} t_1\right) \right|_{\varepsilon=\pi}^2 = 1, \text{ or (with } \cos \frac{\alpha}{2} = c \text{ and } \sin \frac{\alpha}{2} = s \text{) that}$$

$$c^4 + s^4 + c^2 s^2 2 \cos 2k\pi = 1.$$

And since $(c^2 + s^2)^2 = c^4 + s^4 + 2c^2 s^2 = 1$, this means $\cos 2k\pi = 1$ or that k must be an integer. In fact k must equal ± 1 because if, for example k was ± 2 , then for $t = t_1 + \pi\hbar/2\mu H$ (or for $\varepsilon = \pi/2$) we would have, by (8.1.8) that

$$\Phi\left(\frac{1'}{2} t \middle| \frac{1'}{2} t_1\right) = \cos^2 \frac{\alpha}{2} e^{\pm i\pi} + \sin^2 \frac{\alpha}{2} e^{\mp i\pi} = -1 = e^{i\pi}$$

and

$$\frac{1'}{2} t_1 \Rightarrow^\pi \frac{1'}{2} t$$

for all (α, β, γ) which contradicts part (ii) of the second property of spinning motion stated in the beginning of section 8.

Since the transformation function $\Phi(\sigma t | \sigma_1 t_1)$ is not related to any wave function so far calculated we are free to choose the sign of k (see section 8 of Chapter I). Following the usual convention we take $k = +1$ and so arrive at the result

$$\Phi(\sigma t | \sigma_1 t_1) = \begin{pmatrix} e^{i\frac{\mu H}{\hbar}(t-t_1)} & 0 \\ 0 & e^{-i\frac{\mu H}{\hbar}(t-t_1)} \end{pmatrix}. \quad (8.1.10)$$

Case of \mathbf{H} in a general direction

Let a general direction be specified by the vector \overrightarrow{OP} from the origin of fixed coordinates O to a point P on the unit sphere and in turn let this vector be specified by spherical polar angles θ and ϕ , θ being the angle between the z axis of the coordinates

and \overline{OP} , and ϕ the angle between the x axis and the projection of \overline{OP} onto the xy plane. Let the magnetic field \mathbf{H} be parallel to OP with a component H in the direction \overline{OP} , H taking any real value (positive or negative or zero).

To find $\Phi(\sigma t|\sigma_1 t_1)$ we make use of the coordinate system O' formed by rotating the base coordinates O through Euler angles $\beta = \phi + \frac{\pi}{2}$, $\alpha = \theta$ and any angle γ . Starting with the wave function $\Phi(\sigma'_1 t_1|\sigma_1 t_1)$ in O' and applying Feynman's law twice, first with respect to a change in time (from t_1 to t) then with respect to a change in coordinates (from O' to O) we have the requirement

$$\Phi(\sigma t|\sigma_1 t_1) = \sum_{\sigma', \sigma'_1} \Phi(\sigma t|\sigma' t) \Phi(\sigma' t|\sigma'_1 t_1) \Phi(\sigma'_1 t_1|\sigma_1 t_1)$$

where the prime indicates a spin component in O' . In the matrix notation, using (5.16) and (8.1.10) this becomes

$$\Phi(\sigma t|\sigma_1 t_1) = \begin{pmatrix} \cos \frac{\alpha}{2} e^{-i\frac{(\beta+\gamma)}{2}} & -i \sin \frac{\alpha}{2} e^{-i\frac{(\beta-\gamma)}{2}} \\ -i \sin \frac{\alpha}{2} e^{i\frac{(\beta-\gamma)}{2}} & \cos \frac{\alpha}{2} e^{i\frac{(\beta+\gamma)}{2}} \end{pmatrix} \begin{pmatrix} e^{i\varepsilon} & 0 \\ 0 & e^{-i\varepsilon} \end{pmatrix} \begin{pmatrix} \cos \frac{\alpha}{2} e^{i\frac{(\beta+\gamma)}{2}} & i \sin \frac{\alpha}{2} e^{-i\frac{(\beta-\gamma)}{2}} \\ i \sin \frac{\alpha}{2} e^{i\frac{(\beta-\gamma)}{2}} & \cos \frac{\alpha}{2} e^{-i\frac{(\beta+\gamma)}{2}} \end{pmatrix}$$

where ε is as in (8.1.7). Multiplying this out and putting $\beta = \phi + \frac{\pi}{2}$ and $\alpha = \theta$ gives

$$\Phi(\sigma t|\sigma_1 t_1) = \begin{pmatrix} \cos^2 \frac{\theta}{2} e^{i\varepsilon} + \sin^2 \frac{\theta}{2} e^{-i\varepsilon} & \frac{1}{2} \sin \theta e^{-i\phi} (e^{i\varepsilon} - e^{-i\varepsilon}) \\ \frac{1}{2} \sin \theta e^{i\phi} (e^{i\varepsilon} - e^{-i\varepsilon}) & \sin^2 \frac{\theta}{2} e^{i\varepsilon} + \cos^2 \frac{\theta}{2} e^{-i\varepsilon} \end{pmatrix}. \quad (8.1.11)$$

So in the matrix notation this is the spin/spin transformation function between two times in the case of a constant uniform magnetic field in any given direction specified by polar angles θ and ϕ .*

* In (8.1.7) H stands for the component of \mathbf{H} in the given direction (θ, ϕ) (rather than the absolute value of \mathbf{H}). So H may be positive or negative, and in (8.1.11) there are two ways to change the sign of \mathbf{H} . We either let $\mathbf{H} \rightarrow -\mathbf{H}$ (so that $\varepsilon \rightarrow -\varepsilon$) or we change θ and ϕ thus: $\theta \rightarrow \pi - \theta$ and $\phi \rightarrow \pi + \phi$ leaving ε the same. We easily confirm that either way changes the RHS of (8.1.11) in the same manner. We note that $\Phi(\sigma t|\sigma_1 t_1)$ in (8.1.11) is a differentiable function of θ, ϕ and H , and therefore is, as required, a differentiable function of \mathbf{H} at least for $\mathbf{H} \neq 0$. If $\mathbf{H} = 0$ a change $d\mathbf{H}$ in \mathbf{H} can be specified by a direction (θ, ϕ) and a value dH or, equivalently by a direction $(\pi - \theta, \pi + \phi)$ and value $-dH$. The corresponding change $d\Phi(\sigma t|\sigma_1 t_1)$ found by differentiating the RHS of (8.1.11)

8.2 Schrödinger's equation for spinning motion in a uniform magnetic field

First suppose the field is constant in time. Under pure knowledge Y of the spinning motion from time t_0 let $\Phi(\sigma t|Y)$ be our wave function at time $t(> t_0)$ in the fixed coordinates O . By Feynman's law

$$\Phi(\sigma t|Y) = \sum_{\sigma_1} \Phi(\sigma t|\sigma_1 t_1) \Phi(\sigma_1 t_1|Y). \quad (8.2.1)$$

for any t and t_1 where we suppose $t_0 < t_1 < t$. To find the Schrödinger equation we differentiate this with respect to t and put t_1 equal to t (or let $t_1 \rightarrow t$). First, using (8.1.11) we find

$$\begin{aligned} \left. \frac{\partial}{\partial t} \Phi(\sigma t|\sigma_1 t_1) \right|_{t_1=t} &= \frac{d\varepsilon}{dt} \frac{\partial}{\partial \varepsilon} \left(\begin{array}{cc} \cos^2 \frac{\theta}{2} e^{i\varepsilon} + \sin^2 \frac{\theta}{2} e^{-i\varepsilon} & \frac{1}{2} \sin \theta e^{-i\phi} (e^{i\varepsilon} - e^{-i\varepsilon}) \\ \frac{1}{2} \sin \theta e^{i\phi} (e^{i\varepsilon} - e^{-i\varepsilon}) & \sin^2 \frac{\theta}{2} e^{i\varepsilon} + \cos^2 \frac{\theta}{2} e^{-i\varepsilon} \end{array} \right) \Bigg|_{\varepsilon=0} \\ &= i \frac{\mu}{\hbar} \left(\begin{array}{cc} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{array} \right) \end{aligned}$$

where $H_z = H \cos \theta$, $H_x = H \sin \theta \cos \phi$ and $H_y = H \sin \theta \sin \phi$ are the Cartesian components of \mathbf{H} . Hence (8.2.1) implies

$$\left. \begin{aligned} i\hbar \frac{\partial \Phi(\frac{1}{2} t|Y)}{\partial t} &= -\mu [H_z \Phi(\frac{1}{2} t|Y) + (H_x - iH_y) \Phi(-\frac{1}{2} t|Y)] \\ i\hbar \frac{\partial \Phi(-\frac{1}{2} t|Y)}{\partial t} &= -\mu [(H_x + iH_y) \Phi(\frac{1}{2} t|Y) - H_z \Phi(-\frac{1}{2} t|Y)] \end{aligned} \right\} \quad (8.2.2)$$

Now (8.2.2) holds for constant \mathbf{H} . But when \mathbf{H} is changing in magnitude and/or direction we expect (8.2.2) to hold true for short times. This is because the manner of switching of σ from $\frac{1}{2}$ to $-\frac{1}{2}$ or from $-\frac{1}{2}$ to $\frac{1}{2}$ during time t to $t + dt$ is not dependent on the time derivatives of \mathbf{H} (first property in section 8) so the problem of finding $\Phi(\sigma t + dt|Y)$ is *similar* to that of finding it when \mathbf{H} is constant, and the phase factor of similarity can only be 1 (c.f. the derivation of the Schrödinger equation for particle orbital motion in a general scalar potential, section 3.2 of Chapter IV). So (8.2.2) is true even if \mathbf{H} is changing in time.

with respect to \mathbf{H} and setting $\mathbf{H} = 0$ gives the same result either way showing $\Phi(\sigma t|\sigma_1 t_1)$ is a differentiable function of \mathbf{H} even at $\mathbf{H} = 0$.

We can rewrite (8.2.2) as

$$i\hbar \frac{\partial \Phi(\sigma t|Y)}{\partial t} = \sum_{\sigma'} H_{\sigma\sigma'} \Phi(\sigma' t|Y) \quad (8.2.3)$$

where

$$H_{\sigma\sigma'} = -\mu [\sigma_{\sigma\sigma'}^x H_x + \sigma_{\sigma\sigma'}^y H_y + \sigma_{\sigma\sigma'}^z H_z] \quad (8.2.4)$$

and in the matrix representation

$$\sigma_{\sigma\sigma'}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_{\sigma\sigma'}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_{\sigma\sigma'}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (8.2.5)$$

the order of the values of σ and σ' as designators of the matrix elements being (as always) the same as their natural order ($\frac{1}{2}$ then $-\frac{1}{2}$).

Alternatively we can write, in the matrix notation,

$$H_{\sigma\sigma'} = -\mu \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix}. \quad (8.2.6)$$

Result (8.2.3) with (8.2.4) is the general Schrödinger equation for spin one-half in a uniform magnetic field possibly changing in magnitude and direction. In (8.2.4) the Hamiltonian is expressed in terms of the Pauli spin matrices (8.2.5), but it can instead be expressed in terms of the operators $\hat{\sigma}_x, \hat{\sigma}_y$ and $\hat{\sigma}_z$ of section 7 which in matrix form differ from the Pauli matrices only in the factor $\frac{1}{2}$. This gives

$$H_{\sigma\sigma'} = -\mu \frac{1}{s} [\hat{\sigma}_x H_x + \hat{\sigma}_y H_y + \hat{\sigma}_z H_z] \quad (8.2.7)$$

where s is the spin (which is of course $\frac{1}{2}$). We can formally write (8.2.7) as

$$H_{\sigma\sigma'} = -\mu \frac{1}{s} \hat{\boldsymbol{\sigma}} \cdot \mathbf{H} \quad (8.2.8)$$

where $\hat{\boldsymbol{\sigma}}$ is the vector operator whose Cartesian components are the operators $\hat{\sigma}_x, \hat{\sigma}_y$ and $\hat{\sigma}_z$ of section 7.*

* Note that $\hat{\boldsymbol{\sigma}}$ is denoted $\hat{\mathbf{s}}$ in [12] (in for example (110.3) of [12]).

8.3 Precession

Referring to section 6, our wave function $\Phi(\sigma t_1 | \frac{1}{2} t_1)$ over σ in O at time t_1 given $\sigma' = \frac{1}{2}$ in O' at time t_1 is, by (6.1), for given angles θ, ϕ and γ

$$\begin{pmatrix} \Phi(\frac{1}{2} t_1 | \frac{1}{2} t_1) \\ \Phi(-\frac{1}{2} t_1 | \frac{1}{2} t_1) \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \sin \frac{\theta}{2} e^{i\frac{\phi}{2}} \end{pmatrix} e^{-i\frac{1}{2}(\gamma + \frac{\pi}{2})}. \quad (8.3.1)$$

And our wave function over σ' in O' is

$$\begin{pmatrix} \Phi'(\frac{1}{2} t_1 | \frac{1}{2} t_1) \\ \Phi'(-\frac{1}{2} t_1 | \frac{1}{2} t_1) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (8.3.2)$$

Now suppose a uniform constant magnetic field H is present in the z direction in O . Then, by the Schrödinger equation (8.2.2) (or by (8.1.10) and Feynman's law connecting the wave functions $\Phi(\sigma t | \frac{1}{2} t_1)$ and $\Phi(\sigma t_1 | \frac{1}{2} t_1)$), we find

$$\begin{pmatrix} \Phi(\frac{1}{2} t | \frac{1}{2} t_1) \\ \Phi(-\frac{1}{2} t | \frac{1}{2} t_1) \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\frac{\phi - 2\mu H(t-t_1)/\hbar}{2}} \\ \sin \frac{\theta}{2} e^{i\frac{\phi - 2\mu H(t-t_1)/\hbar}{2}} \end{pmatrix} e^{-i\frac{1}{2}(\gamma + \frac{\pi}{2})} \quad (8.3.3)$$

for our wave function in O at a later time t . Changing the Euler angle ϕ thus:

$$\phi \rightarrow \phi + 2\mu H(t - t_1)/\hbar \quad (8.3.4)$$

leaving the angles θ and γ the same, we see that the RHS of (8.3.3) returns to the RHS of (8.3.1), from which we deduce that

$$\begin{pmatrix} \Phi'(\frac{1}{2} t | \frac{1}{2} t_1) \\ \Phi'(-\frac{1}{2} t | \frac{1}{2} t_1) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (8.3.5)$$

applies in the new O' coordinates (just as (8.3.2) followed from (8.3.1) in the original coordinates). So the spin is in precession about the z axis of O . More precisely, on constantly changing ϕ in accordance with (8.3.4), we can say that ' $\sigma' = \frac{1}{2}$ at time t_1 ' implies ' $\sigma' = \frac{1}{2}$ at any later time t ' with phase of implication zero. And it will clearly not affect this implication (except with regard to the value of its determinate phase) if we

choose (alongside the change (8.3.4) in ϕ) to change the angle γ in any definite way. Because the phase of implication is here determinate, the precession is a natural precession. It occurs, whenever the constant uniform magnetic field is present, independently of whatever knowledge we may or may not hold regarding the spinning motion. And under any general state of knowledge of that motion, for any particular value of θ and ϕ , we will (in repeated trials) expect the value of σ' at time t_1 to be sometimes $+\frac{1}{2}$ and sometimes $-\frac{1}{2}$, but in each trial the precessions of the various z' components of spin for different values of θ and ϕ will always take place simultaneously in the same direction and at the same rate.

Similarly we can show that whenever $\sigma' = -\frac{1}{2}$ at time t_1 , $\sigma' = -\frac{1}{2}$ at any later time t provided ϕ is constantly changed in the same manner (i.e. as in (8.3.4)). So when $\sigma' = -\frac{1}{2}$ the precession occurs in the same direction* and at the same rate.

A more general natural precession is present (see p 10-17 of [7]) even when the magnetic field changes smoothly in magnitude and direction. For let the z axis of O be taken initially in the direction of $\mathbf{H}(t)$ (so that $\mathbf{H}(t_1) = H(t_1)\mathbf{k}$) and suppose the spin component in a direction specified by polar angles (θ, ϕ) in O is known to be $+\frac{1}{2}$ at time t_1 . Then our wave function in O at t_1 is

$$\begin{pmatrix} \Phi(\frac{1}{2}t_1 | \frac{1}{2}t_1) \\ \Phi(-\frac{1}{2}t_1 | \frac{1}{2}t_1) \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \sin \frac{\theta}{2} e^{i\frac{\phi}{2}} \end{pmatrix} e^{-i\frac{1}{2}(\gamma+\pi)} \quad (8.3.6)$$

(as in (8.3.1)). In a short time from $t = t_1$ to $t = t_1 + dt$ we know, from our study of precession in a constant magnetic field, that this wave function evolves in a way that implies the spin component in the direction (θ, ϕ) remains equal to $+\frac{1}{2}$ provided ϕ is continually updated according to (8.3.4) leaving θ and γ the same. The small change in $\mathbf{H}(t)$ during the period t_1 to $t_1 + dt$ does not invalidate this argument because it produces only a second order change in the wave function (8.3.3). Therefore ' $\sigma' = \frac{1}{2}$ at time t_1 ' implies ' $\sigma' = \frac{1}{2}$ at time $t_1 + dt$ ' still with a determinate phase of implication so the precession is a natural precession from time t_1 to time $t_1 + dt$. At the end of that time $\mathbf{H}(t)$ will have changed to $\mathbf{H}(t_1 + dt)$, but by turning coordinates O so that $\mathbf{H}(t_1 + dt)$ is back in the z direction we may repeat the same argument. So when the spin component in a given direction specified by polar angles (θ, ϕ) in the original coordinates O is

* Looked at in the classical way, both the spin angular momentum $\sigma'\hbar\mathbf{k}'$ (\mathbf{k}' being the unit vector in the z' direction) and the couple $\mathbf{m} \times \mathbf{H}$ arising from the magnetic moment $\mathbf{m} = \frac{\sigma'}{s}\mu\mathbf{k}'$ have changed sign so it is not surprising that the direction of the precession remains the same when σ' changes sign.

known to be $+\frac{1}{2}$ at time t_1 , thereafter a natural precession takes place about the moving direction of $\mathbf{H}(t)$ and at the (changing) rate of $2\mu|\mathbf{H}(t)|/\hbar$ radians per unit time. If we know initially that the spin component is $-\frac{1}{2}$ rather than $+\frac{1}{2}$ then precession occurs in the same sense and always at the same rate as before.

9. Orbital and spinning motion of a particle in a non-uniform magnetic field

We now consider the orbital and spinning motion of a particle with spin one-half and magnetic moment μ under the action of a generally non-uniform and time dependent magnetic field $\mathbf{H}(\mathbf{r}, t)$. We suppose general time dependent scalar and vector particle potentials $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ may also be acting and in general the particle may possess a charge q as well as a magnetic moment.

9.1 Case of a constant magnetic field and constant net potentials

We consider first the case of a *uniform* and *time independent* magnetic field and *uniform* and *time independent* net scalar and vector potential fields.

The magnetic field must of course result from an electromagnetic vector potential field \mathbf{A}_{em} with the magnetic field \mathbf{H} given by

$$\mathbf{H} = \nabla \times \mathbf{A}_{\text{em}}$$

and to ensure \mathbf{H} is time independent and uniform we make \mathbf{A}_{em} (i) time independent, (ii) everywhere parallel to itself (iii) constant in the direction of itself and (iv) linearly increasing in a direction perpendicular to itself.

Now if the particle has a non-zero charge q it will experience the non-uniform vector potential $q\mathbf{A}_{\text{em}}/c$, so in order that the *net* vector potential be made uniform we need to cancel the effect of the non-uniform electromagnetic potential and this we can do by adding a *non electromagnetic* potential \mathbf{A}_{add} of value $\mathbf{A}_{\text{add}} = -q\mathbf{A}_{\text{em}}/c$. We may then add any uniform and time independent potentials V and \mathbf{A} we choose.*

Under these conditions we claim that the sample spaces S_σ and S_r (of propositions relating to the spinning motion and orbital motion respectively) are (separately) closed. We are able to say this because we know that the potential V and the net potential \mathbf{A} have no effect on the spinning motion and in particular no effect that might depend on the particle's position in space or on the properties of its orbital motion. And we claim the magnetic field \mathbf{H} has no effect on the orbital motion and in particular

* Note that even if the magnetic field is non-uniform and time dependent it is still possible to eliminate the electromagnetic vector potential associated with it by adding an appropriate non-electromagnetic vector potential. The magnetic field, scalar potential and net vector potential experienced by a particle may therefore be quite general and independent of one another.

no effect that might depend on the z component of the particle's spin.* Also, since the magnetic field is uniform its effect on the spinning motion is independent of the position occupied by the particle.

Working in a fixed Cartesian coordinate system O , the position-spin/position-spin transformation function $\phi_{\sigma_1 r_1 t_1}(\sigma r t)$ will be the product of the position/position transformation function $\phi_{r_1 t_1}(\mathbf{r} t)$ in S_r from position \mathbf{r}_1 at time t_1 to position \mathbf{r} at time t and the spin/spin transformation function $\Phi(\sigma t | \sigma_1 t_1)$ from σ_1 at time t_1 to σ at time t (see section 5 of Chapter II). The position/position transformation function in S_r is given by (4.1.18) of Chapter IV. Putting in the known values of $\alpha, \varepsilon, \beta$ and γ , and replacing $\mathbf{r}_2 t_2$ by $\mathbf{r} t$ this is

$$\phi_{r_1 t_1}(\mathbf{r} t) = \left(\frac{2i\pi\hbar}{m}(t-t_1)\right)^{-3/2} \exp i\left(\frac{m(\mathbf{r}-\mathbf{r}_1)^2}{2\hbar(t-t_1)} + \frac{1}{\hbar} \mathbf{A} \cdot (\mathbf{r}-\mathbf{r}_1) - \frac{V}{\hbar}(t-t_1)\right). \quad (9.1.1)$$

The spin/spin transformation function $\Phi(\sigma t | \sigma_1 t_1)$ in sample space S_σ is given by (8.1.11). In the combined sample space $S_r S_\sigma$ the position-spin/position-spin transformation function $\phi_{\sigma_1 r_1 t_1}(\sigma r t)$ is therefore

$$\phi_{\sigma_1 r_1 t_1}(\sigma r t) = \phi_{r_1 t_1}(\mathbf{r} t) \Phi(\sigma t | \sigma_1 t_1) \quad (9.1.2)$$

and we have the following (Feynman Law) relation between the wave functions $\psi_\sigma(\mathbf{r}, t)$ at different times.

$$\psi_\sigma(\mathbf{r}, t) = \sum_{\sigma_1} \int \phi_{\sigma_1 r_1 t_1}(\sigma r t) \psi_{\sigma_1}(\mathbf{r}_1, t_1) d^3 r_1 \quad (9.1.3)$$

Now in (9.1.2) $\phi_{r_1 t_1}(\mathbf{r} t)$ (as given by (9.1.1)) satisfies the Schrödinger equation (4.2.4) of Chapter IV. Also $\Phi(\sigma t | \sigma_1 t_1)$ satisfies the Schrödinger equation (8.2.3). As a result $\phi_{\sigma_1 r_1 t_1}(\sigma r t)$ satisfies the Schrödinger equation

* It might be thought that (as in classical physics) \mathbf{H} and the spin $s = \frac{1}{2}$ should give rise to an effective (generally position dependent) potential energy of order $-\mu\mathbf{H}$ and therefore that \mathbf{H} must affect the orbital motion (as any potential -including any constant potential- always does in quantum mechanics). However it is clear that this (magnetic) potential energy belongs not to the orbital motion but to the spinning motion as is evident from the form of the Hamiltonian (8.2.4) in the Schrödinger equation (8.2.3) for spinning motion in a magnetic field. The absence of a magnetic potential in the orbital motion is related to the classical observation made by Deissler in [25] to the effect that when a classical magnetic dipole moves in a non-uniform magnetic field the magnetic field performs no work on it.

$$\begin{aligned}
 -\frac{\hbar}{i} \frac{\partial \psi_\sigma}{\partial t} = \sum_\sigma \left\{ -\mu \left[\sigma_{\sigma\sigma'}^x H_x + \sigma_{\sigma\sigma'}^y H_y + \sigma_{\sigma\sigma'}^z H_z \right] \right. \\
 \left. + \delta_{\sigma\sigma'} \left(-\frac{\hbar^2}{2m} \nabla^2 + V + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla + \frac{1}{2m} A^2 \right) \right\} \psi_\sigma
 \end{aligned} \tag{9.1.4}$$

as can be checked by substituting $\psi_\sigma(\mathbf{r}, t) = \phi_{\sigma, r t_1}(\mathbf{r}t) \Phi(\sigma t | \sigma_1 t_1)$ in (9.1.4). Being a linear combination of the $\phi_{\sigma, r t_1}(\sigma \mathbf{r}t)$, any wave function $\psi_\sigma(\mathbf{r}, t)$ also satisfies (9.1.4). So in a short time t to $t + dt$

$$\begin{aligned}
 \psi_\sigma \rightarrow \psi_\sigma + \frac{-i}{\hbar} \sum_\sigma \left\{ -\mu \left[\sigma_{\sigma\sigma'}^x H_x + \sigma_{\sigma\sigma'}^y H_y + \sigma_{\sigma\sigma'}^z H_z \right] \right. \\
 \left. + \delta_{\sigma\sigma'} \left(-\frac{\hbar^2}{2m} \nabla^2 + V + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla + \frac{1}{2m} A^2 \right) \right\} \psi_\sigma \cdot dt
 \end{aligned} \tag{9.1.5}$$

9.2 General case of variable and non-uniform magnetic field and potentials

We can now show (9.1.4) is valid when \mathbf{A} , V and \mathbf{H} are any functions of position and time. This is done in the same way as has been done previously (for example in the case of the Schrödinger equation for a variable and non-uniform scalar potential (section 3.2 of Chapter IV)). To be thorough we go through the argument again.

First we note that sample spaces S_σ and S_r are now not separately closed, and it is generally possible to hold a pure state of knowledge only in their combination $S_{\sigma r}$ (see comments made in section 1).

Now suppose we hold pure knowledge Y in $S_{\sigma r}$ relating to both the particle's spinning and orbital motion from which we can infer that a particular wave function $\psi_\sigma(\mathbf{r}, t)$ applies at time t . Suppose, knowing $\psi_\sigma(\mathbf{r}, t)$ everywhere (for all σ) at time t , we wish to calculate (for each σ) $\psi_\sigma(\mathbf{r}, t)$ inside a small volume element dV any short time dt later. For this purpose we form the sample space $S'_{\sigma r}$ of propositions regarding particle orbital motion and spin from time t onwards.

We know, from the first law of potential action (section 3.2 of Chapter III), that the orbital motion of the particle between times t and $t + dt$, should it be in dV at that time, is affected by the potentials $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ in dV between times t and $t + dt$, but not by the spatial or temporal derivatives of $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ in dV between times t and $t + dt$ (nor therefore by the magnetic field $\mathbf{H}(\mathbf{r}, t)$ between times t and $t + dt$ since $\mathbf{H}(\mathbf{r}, t)$ is a function only of the spacial derivatives of the electromagnetic part of the vector potential) nor by the potentials $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ anywhere at future times. It may be affected by the potentials $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ (but not $\mathbf{H}(\mathbf{r}, t)$) at points the particle might have occupied at *earlier* times, but since we have pure knowledge Y in

$S'_{\sigma'}$ (expressed by $\psi_{\sigma}(\mathbf{r},t)$ at time t), knowledge of $V(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$ at earlier times is redundant (see section 3.2 of Chapter I).

We also assume, as a generalisation of the first property of spinning motion in a *uniform* magnetic field (section 8), that the spinning motion of the particle between times t and $t+dt$, should it be in dV at that time, may be affected by the magnetic field $\mathbf{H}(\mathbf{r},t)$ in dV between times t and $t+dt$, but not by the spatial or temporal derivatives of $\mathbf{H}(\mathbf{r},t)$ in dV nor by $\mathbf{H}(\mathbf{r},t)$ anywhere at future times (nor of course by the potentials $V(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$ anywhere at any time). The spinning motion may be affected by the magnetic field $\mathbf{H}(\mathbf{r},t)$ at points the particle might have occupied at *earlier* times, but since we have pure knowledge Y in $S'_{\sigma'}$ (expressed by $\psi_{\sigma}(\mathbf{r},t)$ at time t), knowledge of $\mathbf{H}(\mathbf{r},t)$ at earlier times is redundant.

We know that the particle does not move infinitely fast so that our knowledge regarding particle position at time t outside some small volume element dV' enclosing dV is, for our purpose, superfluous. Therefore our problem is *similar* to the one in which the potentials and magnetic field are constant in time and space and equal to their values at the position of dV and at the time t in question. In that case (9.1.5) holds for the change in $\psi_{\sigma}(\mathbf{r},t)$ over any short enough time. So by the similarity principle, for \mathbf{r} in dV and after any short enough time dt

$$\psi_{\sigma}(\mathbf{r},t+dt) = \left(\psi_{\sigma}(\mathbf{r},t) + \frac{-i}{\hbar} \sum_{\sigma'} \left\{ -\mu [\sigma_{\sigma\sigma'}^x H_x + \sigma_{\sigma\sigma'}^y H_y + \sigma_{\sigma\sigma'}^z H_z] \right. \right. \\ \left. \left. + \delta_{\sigma\sigma'} \left(-\frac{\hbar^2}{2m} \nabla^2 + V + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla + \frac{1}{2m} A^2 \right) \right\} \psi_{\sigma'} dt \right) e^{i\beta}$$

where β is a real constant independent of dt . But for $dt \rightarrow 0$ we must have $\psi_{\sigma}(\mathbf{r},t+dt) = \psi_{\sigma}(\mathbf{r},t)$ so that β can only be zero and $\psi_{\sigma}(\mathbf{r},t)$ must satisfy the differential equation (9.1.4) in any short enough time interval. Being valid for any short enough time interval, and in any volume element dV , (9.1.4) is valid for all times and positions in space and we have established the Schrödinger equation for a spinning and orbiting particle moving under the action of generally non-uniform and time dependent scalar and vector potentials and a generally non-uniform and time dependent magnetic field.

CHAPTER VIII

PAIRS OF SPIN ONE-HALF SYSTEMS, SPIN ONE AND SPIN ZERO

1. Total spin of a pair of spin one-half systems

Consider a pair of distinguishable systems each having spin one-half over a time period. The systems may be experiencing one and the same uniform (possibly time-dependent) magnetic field but we assume there is no interaction between their spins.* Let us label these systems 1 and 2. Their spin values are denoted s_1 and s_2 respectively with $s_1 = s_2 = 1/2$. The propositions ‘ $\sigma_1\sigma_2$ ’ claiming system 1 has a z component of spin σ_1 relative to a fixed Cartesian coordinate system O and system 2 has a z component of spin σ_2 relative to the same coordinates constitute a basis in the closed sample space $S_{\sigma_1\sigma_2}$ which is the combination $S_{\sigma_1}S_{\sigma_2}$ of the closed sample spaces S_{σ_1} and S_{σ_2} (of type S_σ in section 1 of Chapter VII) of the separate systems. The sample space $S_{\sigma_1\sigma_2}$ and the propositions ‘ $\sigma_1\sigma_2$ ’ relate to ‘a pair of spin one-half systems’. Supposing system 1 comes before system 2 in the natural order of systems (see section 3.6 of Chapter III), we claim that the discrete basis ‘ $\sigma_1\sigma_2$ ’ of the pair of spin one-half systems has a natural order given by†

$$\sigma_1\sigma_2 = \frac{1}{2} \frac{1}{2}, \frac{1}{2} \frac{-1}{2}, -\frac{1}{2} \frac{1}{2}, -\frac{1}{2} \frac{-1}{2}. \quad (1.1)$$

It is clear that a natural order for the propositions of this basis cannot be claimed without the assumption of a natural order of the subsystems themselves.‡

Now the pair of spin one-half systems also has a property called ‘total spin’. This is characterised by the following variables, (i) a spin s switching from time to time from one to another of the values $|s_1 \pm s_2|$ (i.e. 1 or 0), and (ii) (generally time dependent) z components of spin σ (in each fixed Cartesian coordinate frame) taking one or other of the values $s, s-1, \dots -s$ (i.e. 0 if $s=0$ but 1, 0 or -1 if $s=1$). The total spin value s (taking value 1 or 0) is coordinate system independent. And the same z component σ of the total spin denotes the same property in all fixed Cartesian coordinate systems of the same orientation occupied in the same way regardless of the positions of their origins.

* Spin/spin interactions (as well as spin/orbit interactions) are best taken to be entirely absent in non-relativistic quantum mechanics.

† This natural order is derived by following the general rule of Kronecker matrix multiplication [31]. So the order in (1.1) is the order of the elements (as normally written) in the developed Kronecker product

$(\frac{1}{2} \frac{-1}{2}) \otimes (\frac{1}{2} \frac{-1}{2}) = (\frac{1}{2} \frac{1}{2}, \frac{1}{2} \frac{-1}{2}, -\frac{1}{2} \frac{1}{2}, -\frac{1}{2} \frac{-1}{2})$ of the single row matrices $(\frac{1}{2} \frac{-1}{2})$ and $(\frac{1}{2} \frac{-1}{2})$ (for the subsystems) whose elements are in the natural order of *their* bases.

‡ If we assumed system 2 came before system 1 in the natural order then we would have to write

$$\sigma_2\sigma_1 = \frac{1}{2} \frac{1}{2}, \frac{1}{2} \frac{-1}{2}, -\frac{1}{2} \frac{1}{2}, -\frac{1}{2} \frac{-1}{2}.$$

VIII. Pairs of spin $\frac{1}{2}$ systems, spin 1 and spin 0

Now we extend the sample space $S_{\sigma_1\sigma_2}$ to include reference to total spin and we claim that propositions ‘ $s\sigma$ ’ constitute another basis (in the extended sample space) having a natural order given by

$$s\sigma = 11, 10, 1-1, 00. \quad (1.2)$$

This natural order applies whether the natural order of the subsystems is assumed to be 1,2 (as we are supposing) or 2,1.

Each subsystem (i.e. each system of spin one-half) will carry its own magnetic moment (say $\mu^{(1)}$ and $\mu^{(2)}$ for subsystem 1 and 2 respectively). And if a uniform magnetic field is present, this will have a bearing on the spinning motion of each subsystem (and therefore on the spinning motion of the whole system). We postulate the following kinematic properties of total spin which hold at any one time so long as the subsystems 1 and 2 are and remain spin one-half systems over the period of time in question.

First property The peculiar nature of the spin one-half subsystems carrying the spins $s_1 = \frac{1}{2}$ and $s_2 = \frac{1}{2}$, and the magnetic moments $\mu^{(1)}$ and $\mu^{(2)}$, has no bearing on the value of the total spin s or on the value of the z component σ of total spin in any fixed Cartesian coordinate system at any time.

Second property In any fixed Cartesian coordinate system at any one time, (i) σ is equal to the sum $\sigma_1 + \sigma_2$ of the values of σ_1 and σ_2 possessed by the subsystems, (ii) The propositions ‘ $\sigma_1\sigma_2 = \frac{1}{2}\frac{1}{2}$ ’ and ‘ $s\sigma = 11$ ’ are fully equivalent, (iii) the propositions ‘ $\sigma_1\sigma_2 = -\frac{1}{2}-\frac{1}{2}$ ’ and ‘ $s\sigma = 1-1$ ’ are fully equivalent, and (iv) the proposition ‘ $s\sigma = 10$ ’ implies the proposition ‘ $\sigma_1\sigma_2 = \frac{1}{2}-\frac{1}{2}$ or $-\frac{1}{2}\frac{1}{2}$ ’ with zero phase of implication.

Third property In any two fixed Cartesian coordinate systems O and O' at any one time the propositions ‘ $s\sigma = 00$ ’ and ‘ $s'\sigma' = 00$ ’ evidently imply one another and they do so with phases of implication equal to zero regardless of the orientations of the coordinate systems or the way they occupy their orientations.

2. Transformation functions between the bases $\sigma_1\sigma_2$ and $s\sigma$

On account of parts (i)-(iii) of the second property claimed in section 1 the transformation functions $\Phi(s\sigma|\sigma_1\sigma_2)$ and $\Phi(\sigma_1\sigma_2|s\sigma)$ at any one time can evidently be written (in matrix form) as

$$\Phi(s\sigma|\sigma_1\sigma_2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & A & C & 0 \\ 0 & 0 & 0 & 1 \\ 0 & B & D & 0 \end{pmatrix}, \quad \Phi(\sigma_1\sigma_2|s\sigma) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & A^* & 0 & B^* \\ 0 & C^* & 0 & D^* \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (2.1)$$

where the rows (numbered top to bottom by $s\sigma$ in the first matrix and by $\sigma_1\sigma_2$ in the second) and the columns (numbered left to right by $\sigma_1\sigma_2$ in the first matrix and by $s\sigma$ in the second) are in the natural order of the propositions of the respective bases, and A, B, C and D are (perhaps complex-valued) constants yet to be found. With no magnetic field present these constants are clearly the same in all fixed Cartesian coordinate systems at all times, regardless of the nature of the spin one-half systems. This follows from the first property above, the isotropy of space, the homogeneity of space and time and the similarity principle and the fact that some of the entries in the matrices are equal to 1 thus fixing the absolute phases of the transformation functions. The constants are also the same in all fixed Cartesian coordinate systems and at all times when a (possibly time-dependent) uniform magnetic field is present because we claim that total spin is (like spin one-half) a property amenable to the principle of short time isolation.*

The required orthonormality of the transformation functions gives

$$AA^* + CC^* = 1, \quad BB^* + DD^* = 1, \quad AB^* + CD^* = 0 \quad (2.2)$$

and phase normalisation gives

$$BC - AD = 1. \quad (2.3)$$

Solving (2.3) and the last of (2.2) for A and C in terms of B and D we easily get to see that

$$C = B^* \quad \text{and} \quad A = -D^* \quad (\text{assuming } B^* \neq 0) \quad (2.4)$$

or if $B^* = 0$ then

$$B^* = C = 0 \quad \text{and} \quad AD = -1. \quad (2.5)$$

* The argument used here is the same as in section 3 of Chapter VII in connection with a single spin one-half system. $\sigma_1\sigma_2$ represents a pure state of knowledge so past history of the magnetic field is redundant. Knowledge of the future magnetic field is redundant because it has no effect on σ_1, σ_2, S or σ . And knowledge of the present magnetic field is redundant because σ_1, σ_2, S and σ are each amenable to the principle of short-time isolation.

This goes part way to finding the constants A, B, C and D . To go further we need to consider rotations of coordinates.

3. Transformation functions under rotation of coordinates

Under a rotation of coordinates from O to O' the transformation function $\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2)$ will be the product of the transformation functions for each subsystem under the same rotation of coordinates:

$$\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2) = \Phi(\sigma'_1|\sigma_1)\Phi(\sigma'_2|\sigma_2)$$

or in matrix notation

$$\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2) = \begin{pmatrix} a^2 & ac & ca & c^2 \\ ab & ad & cb & cd \\ ba & bc & da & dc \\ b^2 & bd & db & d^2 \end{pmatrix} \quad (3.1)$$

where a, b, c and d are given by (5.16) of Chapter VII.*

Now Feynman's law (twice applied) requires that the transformation function $\Phi(s'\sigma'|s\sigma)$ satisfies

$$\Phi(s'\sigma'|s\sigma) = \sum_{\sigma'_1\sigma'_2} \sum_{\sigma_1\sigma_2} \Phi(s'\sigma'|\sigma'_1\sigma'_2)\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2)\Phi(\sigma_1\sigma_2|s\sigma)$$

or in the matrix notation

$$\Phi(s'\sigma'|s\sigma) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & A & C & 0 \\ 0 & 0 & 0 & 1 \\ 0 & B & D & 0 \end{pmatrix} \begin{pmatrix} a^2 & ac & ca & c^2 \\ ab & ad & cb & cd \\ ba & bc & da & dc \\ b^2 & bd & db & d^2 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & A^* & 0 & B^* \\ 0 & C^* & 0 & D^* \\ 0 & 0 & 1 & 0 \end{pmatrix}. \quad (3.2)$$

Multiplying this product out we obtain for the last column the result

* With our method of ordering rows and columns according to the natural order of the bases, matrix $\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2)$ is the Kronecker product [31] of the matrices $\Phi(\sigma'_1|\sigma_1)$ and $\Phi(\sigma'_2|\sigma_2)$. The determinant of a Kronecker product $\mathbf{A} \otimes \mathbf{B}$ of an $n \times n$ matrix \mathbf{A} and a $p \times p$ matrix \mathbf{B} is given by $|\mathbf{A} \otimes \mathbf{B}| = |\mathbf{A}|^p |\mathbf{B}|^n$ (see p.709 of [31]) so $\det[\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2)] = 1$ as required of any ordered discrete basis (see (3.4.2) of Chapter 1).

$$\Phi(s'\sigma'|00) = \begin{pmatrix} acB^* + caD^* \\ A(adB^* + cbD^*) + C(bcB^* + daD^*) \\ bdB^* + dbD^* \\ B(adB^* + cbD^*) + D(bcB^* + daD^*) \end{pmatrix}. \quad (3.3)$$

But by the third property of total spin ' $s\sigma = 00$ ' implies ' $s'\sigma' = 00$ ' with phase of implication zero. Hence

$$\Phi(s'\sigma'|00) = \delta_{s'\sigma',00}$$

Therefore all elements but the last in column (3.3) must be zero while the last itself is 1. Making use of the second of results (2.2) we can now rule out the possibility of (2.5) because it would make the bottom element in (3.3) equal to da which is certainly not equal to 1 for all angles of rotation. Using (2.4) and the fact that the top element in (3.3) is zero we thus establish that $B^* = -D^* = A$. We therefore have, by (2.4), that $A = C$ and the second of (2.1) becomes

$$\Phi(\sigma_1\sigma_2|s\sigma) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & A^* & 0 & A \\ 0 & A^* & 0 & -A \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (3.4)$$

Putting $s\sigma = 10$ and applying the sum rule (3.4.9) of Chapter I we get

$$\Phi(\frac{1}{2} - \frac{1}{2} \text{ or } -\frac{1}{2} \frac{1}{2} | 10) = \sqrt{2}\Phi(\frac{1}{2} - \frac{1}{2} | 10) = \sqrt{2}A^*.$$

But, by part (iv) of the second property in section 1, $\sqrt{2}A^*$ must equal 1. So A must equal $1/\sqrt{2}$ and we arrive at

$$\Phi(s\sigma|\sigma_1\sigma_2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \end{pmatrix} \quad (3.5)$$

for the first of the transformation functions (2.1) in matrix form. From (3.2) it follows that

$$\Phi(s'\sigma'|s\sigma) = \begin{pmatrix} a^2 & \sqrt{2}ac & c^2 & 0 \\ \sqrt{2}ab & ad+bc & \sqrt{2}cd & 0 \\ b^2 & \sqrt{2}bd & d^2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (3.6)$$

This is the matrix form of the $s\sigma$ transformation function under coordinate rotation.

4. Pair of spin one-half systems in a uniform magnetic field

Pure knowledge Y over the sample space $S_{\sigma_1\sigma_2}$ of a pair of spin one-half systems in a (possibly time dependent) uniform magnetic field can be expressed as a wave function $\Phi(\sigma_1\sigma_2t|Y)$ of the z components of spin at any time t during the time period covered by $S_{\sigma_1\sigma_2}$. This wave function is related to the wave function $\Phi(\sigma_1\sigma_2t'|Y)$ of the spin components at an earlier time t' during evolution in the magnetic field. Either wave function can serve to represent the pure knowledge Y . The relation between them is of course

$$\Phi(\sigma_1\sigma_2t|Y) = \sum_{\sigma'_1\sigma'_2} \Phi(\sigma_1\sigma_2t|\sigma'_1\sigma'_2t')\Phi(\sigma'_1\sigma'_2t'|Y) \quad (4.1)$$

the transformation function $\Phi(\sigma_1\sigma_2t|\sigma'_1\sigma'_2t')$ being given by

$$\Phi(\sigma_1\sigma_2t|\sigma'_1\sigma'_2t') = \Phi(\sigma_1t|\sigma'_1t')\Phi(\sigma_2t|\sigma'_2t'), \quad (4.2)$$

where the functions on the RHS are the transformation functions for each subsystem in the magnetic field. We have seen that the latter transformation functions satisfy the Schrödinger equation ((8.2.3) of Chapter VII) so we can write for either subsystem

$$i\hbar \frac{\partial \Phi(\sigma t|\sigma' t')}{\partial t} = \sum_{\sigma''} H_{\sigma\sigma''} \Phi(\sigma'' t|\sigma' t')$$

where

$$H_{\sigma\sigma''} = -\mu \left[\sigma_{\sigma\sigma''}^x H_x + \sigma_{\sigma\sigma''}^y H_y + \sigma_{\sigma\sigma''}^z H_z \right]$$

μ being the magnetic moment of the subsystem in question.

As we can check by direct substitution, the transformation function $\Phi(\sigma_1\sigma_2t|\sigma'_1\sigma'_2t')$ given by (4.2) satisfies the Schrödinger equation

$$i\hbar \frac{\partial \Phi(\sigma_1 \sigma_2 t | \sigma'_1 \sigma'_2 t')}{\partial t} = \sum_{\sigma_1 \sigma_2} (H_{\sigma_1 \sigma_1}^{(1)} \delta_{\sigma_2 \sigma_2} + \delta_{\sigma_1 \sigma_1} H_{\sigma_2 \sigma_2}^{(2)}) \Phi(\sigma_1 \sigma_2 t | \sigma'_1 \sigma'_2 t') \quad (4.3)$$

where

$$H_{\sigma_1 \sigma_1}^{(1)} = -\mu^{(1)} [\sigma_{\sigma_1 \sigma_1}^x H_x + \sigma_{\sigma_1 \sigma_1}^y H_y + \sigma_{\sigma_1 \sigma_1}^z H_z]$$

$$H_{\sigma_2 \sigma_2}^{(2)} = -\mu^{(2)} [\sigma_{\sigma_2 \sigma_2}^x H_x + \sigma_{\sigma_2 \sigma_2}^y H_y + \sigma_{\sigma_2 \sigma_2}^z H_z]$$

are the Hamiltonians for the subsystems 1 and 2 respectively. Being a linear combination of the $\Phi(\sigma_1 \sigma_2 t | \sigma'_1 \sigma'_2 t')$ (as in (4.1)), any wave function $\Phi(\sigma_1 \sigma_2 t | Y)$ also satisfies the Schrödinger equation (4.3), i.e.

$$i\hbar \frac{\partial \Phi(\sigma_1 \sigma_2 t | Y)}{\partial t} = \sum_{\sigma_1 \sigma_2} H_{\sigma_1 \sigma_2, \sigma_1 \sigma_2} \Phi(\sigma_1 \sigma_2 t | Y) \quad (4.4)$$

where

$$H_{\sigma_1 \sigma_2, \sigma_1 \sigma_2} = H_{\sigma_1 \sigma_1}^{(1)} \delta_{\sigma_2 \sigma_2} + \delta_{\sigma_1 \sigma_1} H_{\sigma_2 \sigma_2}^{(2)} \quad (4.5)$$

We can express the Hamiltonian $H_{\sigma_1 \sigma_2, \sigma_1 \sigma_2}$ in 4×4 matrix form with the rows following (from top to bottom) the natural order (1.1) of the basis $\sigma_1 \sigma_2$ and the columns following (from left to right) the natural order of the basis $\sigma'_1 \sigma'_2$. This is accomplished by representing $H_{\sigma_1 \sigma_1}^{(1)}$ and $H_{\sigma_2 \sigma_2}^{(2)}$, and $\delta_{\sigma_2 \sigma_2}$ and $\delta_{\sigma_1 \sigma_1}$ by 2×2 matrices (with their rows and columns following the natural order of *their* bases) and writing (4.5) in the matrix form

$$H_{\sigma_1 \sigma_2, \sigma_1 \sigma_2} = H_{\sigma_1 \sigma_1}^{(1)} \otimes \delta_{\sigma_2 \sigma_2} + \delta_{\sigma_1 \sigma_1} \otimes H_{\sigma_2 \sigma_2}^{(2)}$$

where \otimes denotes the Kronecker product (as defined for example in [31]). Then by (8.2.6) of Chapter VII

$$\begin{aligned} H_{\sigma_1 \sigma_1}^{(1)} \otimes \delta_{\sigma_2 \sigma_2} &= -\mu^{(1)} \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= -\mu^{(1)} \begin{pmatrix} H_z & 0 & H_x - iH_y & 0 \\ 0 & H_z & 0 & H_x - iH_y \\ H_x + iH_y & 0 & -H_z & 0 \\ 0 & H_x + iH_y & 0 & -H_z \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} \delta_{\sigma_1\sigma'_1} \otimes H_{\sigma_2\sigma'_2}^{(2)} &= -\mu^{(2)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix} \\ &= -\mu^{(2)} \begin{pmatrix} H_z & H_x - iH_y & 0 & 0 \\ H_x + iH_y & -H_z & 0 & 0 \\ 0 & 0 & H_z & H_x - iH_y \\ 0 & 0 & H_x + iH_y & -H_z \end{pmatrix} \end{aligned}$$

Adding the two gives

$$H_{\sigma_1\sigma_2,\sigma'_1\sigma'_2} = - \begin{pmatrix} (\mu^{(1)} + \mu^{(2)})H_z & \mu^{(2)}(H_x - iH_y) & \mu^{(1)}(H_x - iH_y) & 0 \\ \mu^{(2)}(H_x + iH_y) & (\mu^{(1)} - \mu^{(2)})H_z & 0 & \mu^{(1)}(H_x - iH_y) \\ \mu^{(1)}(H_x + iH_y) & 0 & (-\mu^{(1)} + \mu^{(2)})H_z & \mu^{(2)}(H_x - iH_y) \\ 0 & \mu^{(1)}(H_x + iH_y) & \mu^{(2)}(H_x + iH_y) & -(\mu^{(1)} + \mu^{(2)})H_z \end{pmatrix} \dots(4.6)$$

To find the Schrödinger equation in the $s\sigma$ representation we substitute for $\Phi(\sigma_1\sigma_2t|Y)$ and $\Phi(\sigma'_1\sigma'_2t|Y)$ in (4.4) using the relation

$$\Phi(\sigma_1\sigma_2t|Y) = \sum_{s\sigma} \Phi(\sigma_1\sigma_2|s\sigma)\Phi(s\sigma t|Y).$$

Multiplying the result by $\Phi(s'\sigma'|\sigma_1\sigma_2)$ and summing over $\sigma_1\sigma_2$ shows that the Schrödinger equation governing the wave function $\Phi(s\sigma t|Y)$ is

$$i\hbar \frac{\partial \Phi(s\sigma t|Y)}{\partial t} = \sum_{s'\sigma'} H_{s\sigma,s'\sigma'} \Phi(s'\sigma' t|Y) \quad (4.7)$$

where

$$H_{s\sigma,s'\sigma'} = \sum_{\sigma_1\sigma_2} \sum_{\sigma'_1\sigma'_2} \Phi(\sigma_1\sigma_2|s\sigma) H_{\sigma_1\sigma_2,\sigma'_1\sigma'_2} \Phi(\sigma'_1\sigma'_2|s'\sigma'). \quad (4.8)$$

Using (3.5) and (4.6) the matrix form of $H_{s\sigma,s'\sigma'}$ is found to be

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$$H_{s\sigma, s'\sigma'} = - \begin{pmatrix} (\mu^{(1)} + \mu^{(2)})H_z & \frac{1}{\sqrt{2}}(\mu^{(1)} + \mu^{(2)})(H_x - iH_y) & 0 & \frac{1}{\sqrt{2}}(\mu^{(2)} - \mu^{(1)})(H_x - iH_y) \\ \frac{1}{\sqrt{2}}(\mu^{(1)} + \mu^{(2)})(H_x + iH_y) & 0 & \frac{1}{\sqrt{2}}(\mu^{(1)} + \mu^{(2)})(H_x - iH_y) & (\mu^{(1)} - \mu^{(2)})H_z \\ 0 & \frac{1}{\sqrt{2}}(\mu^{(1)} + \mu^{(2)})(H_x + iH_y) & -(\mu^{(1)} + \mu^{(2)})H_z & \frac{1}{\sqrt{2}}(\mu^{(1)} - \mu^{(2)})(H_x + iH_y) \\ \frac{1}{\sqrt{2}}(\mu^{(2)} - \mu^{(1)})(H_x + iH_y) & (\mu^{(1)} - \mu^{(2)})H_z & \frac{1}{\sqrt{2}}(\mu^{(1)} - \mu^{(2)})(H_x - iH_y) & 0 \end{pmatrix} \quad (4.9)$$

4.1 The case when the magnetic moments $\mu^{(1)}$ and $\mu^{(2)}$ are equal

When $\mu^{(1)} = \mu^{(2)}$ the Hamiltonian in (4.9) simplifies to

$$H_{s\sigma, s'\sigma'} = -\mu \begin{pmatrix} H_z & \frac{1}{\sqrt{2}}(H_x - iH_y) & 0 & 0 \\ \frac{1}{\sqrt{2}}(H_x + iH_y) & 0 & \frac{1}{\sqrt{2}}(H_x - iH_y) & 0 \\ 0 & \frac{1}{\sqrt{2}}(H_x + iH_y) & -H_z & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (4.1.1)$$

where $\mu = \mu^{(1)} + \mu^{(2)}$.

If knowledge Y is knowledge expressed as ‘ $s\sigma=00$ at time t_1 ’ or as ‘ $00t_1$ ’, where ‘ $s\sigma t$ ’ is the proposition claiming total spin s and z component of total spin σ are present at time t , then clearly $\Phi(s\sigma t_1|Y) = \delta_{s\sigma, 00}$, or in vector form

$$\Phi(s\sigma t_1|Y) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

And when the Hamiltonian has the form (4.1.1) with its bottom row a row of zeros, we have, by (4.7), that at time $t_1 + dt$ the wave function is

$$\Phi(s\sigma t_1 + dt|Y) = \Phi(s\sigma t_1|Y) + \frac{1}{i\hbar} \sum_{s'\sigma'} H_{s\sigma, s'\sigma'} \Phi(s'\sigma' t_1|Y) dt = \Phi(s\sigma t_1|Y).$$

So it is clear that the wave function does not change in time. And at any time t

$$\Phi(s\sigma t|Y) = \delta_{s\sigma, 00}$$

or ‘ $s\sigma=00$ at time t_1 ’ \Leftrightarrow ‘ $s\sigma=00$ at time t ’ telling us that the state of total spin $s=0$ is a property naturally conserved independently of our knowledge of the spin dynamics.

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So a pair of spin one-half systems with equal magnetic moments in a uniform (possibly time dependent) magnetic field has a total spin s which remains constant in time independently of any knowledge we may or may not hold in relation to the spinning motion. For whenever $s=0$ at one time then $s=0$ at any other time as we have seen. And whenever $s=1$ at one time then it must be that $s=1$ at any other time, for if s were zero at that other time it would have had to have been zero at the original time too, contrary to hypothesis.

Put another way, a pair of spin one-half systems with equal magnetic moments in a uniform magnetic field (possible time-dependent) constitute either a ‘spin 1 system’ or a ‘spin 0 system’ independently of our knowledge of the system spin dynamics. And if we have sufficient knowledge (which need not always be pure knowledge) of the system spin dynamics to be aware the system is a spin 1 system (or a spin 0 system) then that awareness can be classified as part of our general knowledge regarding the unchanging properties of the system.

5. Spin one systems

The nature of spin one is covered in section 1 of Chapter VII if we take s to equal 1 in that section. Nonetheless we review the specific nature of spin one systems and note two properties that relate to them.

We may claim to know that some systems of particles (including some single particles) are ‘spin 1 systems’. They are then understood to have a spin of magnitude one and a constant magnetic moment μ –both constant over a certain time period under certain conditions *or* constant for all time in the case of single particles.

Spin one is a dynamical property characterised by a dimensionless spin value s ($=1$). A spin one system has a dimensionless (generally time dependent) ‘ z component of spin’ σ relative to a fixed Cartesian coordinate reference frame. At any one time and in any one such frame, σ has one of the discrete values $s, s-1, \dots, -s$ (i.e. 1, 0 or -1) representing a property of the system in that frame. A definite z component of spin (e.g. $\sigma=1$) in each coordinate system of different orientation (or the same orientation occupied the other way) represents a different property. But the same z components of spin in fixed coordinate systems that differ only by a simple *translation* in space, represent the *same* property.

All propositions concerning the z components of spin in fixed Cartesian coordinate systems over a time period constitute a complete sample space S_σ . The three propositions claiming one or other value of the z component of spin σ relative to a particular fixed Cartesian coordinate system at a certain time constitute a basis in S_σ , the natural order of the propositional basis being always given by the following order of the σ values claimed.

$$\sigma = 1, 0, -1. \tag{5.1}$$

VIII. Pairs of spin $\frac{1}{2}$ systems, spin 1 and spin 0

Wave functions for spin using such a basis are normalised (complex valued) probability distributions $\psi(\sigma)$ over the (three) possible values of σ .

With regard to a system of spin one, let the z component of spin relative to a fixed Cartesian coordinate frame O be σ and let the z component of spin relative to another fixed Cartesian coordinate frame O' sharing its origin with O be σ' . (Of course $s (=1)$ is itself independent of the coordinate frame.) We again specify the state of O' relative to O using Euler angles α, β and γ , as in section 2 of Chapter VII.

Transformation functions and the Schrödinger equation for a system known to be a system of spin one over a time period are most easily derived using the following assumed properties in relation to systems of spin one.

First property The nature of the system carrying the spin $s=1$ and magnetic moment μ has no bearing on the values of its z components of spin in O and O' (or in any fixed coordinate frame) over the time period.

Second property When a system made up of two distinguishable spin one-half subsystems 1 and 2 with equal magnetic moments is in a uniform (possibly time dependent) magnetic field and is prepared in a way that ensures its total spin s is known to be 1 over a time period, then (i) the system is a spin one system during that time period, (ii) its z component of spin σ in any fixed coordinate frame is at any time equal to the sum of the z components of spin of the subsystems 1 and 2 in the same coordinate frame, and (iii) its magnetic moment is the sum of the magnetic moments of the subsystems 1 and 2.

5.1 Spin/spin transformation functions

From the above properties, the problem of finding the probabilities $\Phi(\sigma|\sigma')$ and $\Phi(\sigma'\sigma)$ (i.e. the spin/spin transformation functions for any spin one system between fixed coordinates O and O' of different orientation) is *similar* to that of finding the probabilities $\Phi(s\sigma|s'\sigma')$ and $\Phi(s'\sigma's\sigma)$ (i.e. the spin/spin transformation functions for a pair of spin one-half systems) when it is known that s (and therefore, by (3.6), also s') is equal to 1. By the similarity principle we may therefore write

$$\Phi(\sigma'\sigma) = \Phi(1\sigma'|1\sigma)e^{i\lambda}$$

where the phase λ is independent of σ and σ' , and of the Euler angles α, β, γ specifying O' relative to O . But with $\alpha = \beta = \gamma = 0$ both $\Phi(\sigma'\sigma)$ and $\Phi(1\sigma'|1\sigma)$ must be $\delta_{\sigma\sigma'}$, so λ can only be zero, and from (3.6) we have

$$\Phi(\sigma'|\sigma) = \begin{pmatrix} a^2 & \sqrt{2}ac & c^2 \\ \sqrt{2}ab & ad + bc & \sqrt{2}cd \\ b^2 & \sqrt{2}bd & d^2 \end{pmatrix} \quad (5.1.1)$$

So this is the spin/spin transformation function for any spin one system under coordinate rotation.

5.2 Spin one system in a uniform magnetic field

Consider the spinning motion of any spin one system of magnetic moment μ in a uniform (possibly time dependent) magnetic field.

Again, because of the two properties of spin one (given in the beginning of section 5), the problem of finding the probabilities $\Phi(\sigma t|\sigma' t')$ (i.e. of finding the wave function of any spin one system at time t knowing σ' in the same coordinate frame at another time t') is *similar* to that of finding the wave function $\Phi(s\sigma t|s'\sigma' t')$ (with $s = s' = 1$) of a pair of spin one-half systems (with magnetic moments $\mu^{(1)}$ and $\mu^{(2)}$ each equal to $\frac{1}{2}\mu$) in a uniform (possibly time dependent) magnetic field at time t knowing σ' at another time t' and knowing $s' = 1$ at time t' (and therefore knowing $s = 1$ at all times). Hence we can write

$$\Phi(\sigma t|\sigma' t') = \Phi(1\sigma t|1\sigma' t')e^{i\lambda}$$

where λ is independent of σ, t, σ' and t' , and can only be zero because both wave functions must reduce to $\delta_{\sigma\sigma'}$ when $t \rightarrow t'$.

But $\Phi(s\sigma t|s'\sigma' t')$ must satisfy the Schrödinger equation (4.7) with $Y = s'\sigma' t'$. To avoid confusion we replace the dummy suffix $s'\sigma'$ on the RHS of (4.7) by $s''\sigma''$, so we can say

$$i\hbar \frac{\partial \Phi(s\sigma t|s'\sigma' t')}{\partial t} = \sum_{s''\sigma''} H_{s\sigma, s''\sigma''} \Phi(s''\sigma'' t|s'\sigma' t') \quad (5.2.1)$$

With $s = s' = 1$, (5.2.1) with (4.1.1) for $H_{s\sigma, s''\sigma''}$ gives

$$i\hbar \frac{\partial \Phi(1\sigma t|1\sigma' t')}{\partial t} = \sum_{\sigma''} H_{1\sigma, 1\sigma''} \Phi(1\sigma'' t|1\sigma' t').$$

Since $\Phi(\sigma t|\sigma' t') = \Phi(1\sigma t|1\sigma' t')$, the wave function $\Phi(\sigma t|\sigma' t')$ satisfies the Schrödinger equation

$$i\hbar \frac{\partial \Phi(\sigma t | \sigma' t')}{\partial t} = \sum_{\sigma''} H_{\sigma\sigma''} \Phi(\sigma'' t | \sigma' t') \quad (5.2.2)$$

where, by (4.1.1)

$$H_{\sigma\sigma'} = H_{1\sigma,1\sigma'} = -\mu \begin{pmatrix} H_z & \frac{1}{\sqrt{2}}(H_x - iH_y) & 0 \\ \frac{1}{\sqrt{2}}(H_x + iH_y) & 0 & \frac{1}{\sqrt{2}}(H_x - iH_y) \\ 0 & \frac{1}{\sqrt{2}}(H_x + iH_y) & -H_z \end{pmatrix} \quad (5.2.3)$$

where $\mu = \mu^{(1)} + \mu^{(2)}$ is, by part (iii) of the second property of spin one systems, the magnetic moment of the system of spin one.

By Feynman's law the general wave function $\Phi(\sigma t | Y)$ for a spin one system under pure knowledge Y satisfies

$$\Phi(\sigma t | Y) = \sum_{\sigma'} \Phi(\sigma t | \sigma' t') \Phi(\sigma' t' | Y),$$

i.e. it is linear combination of the wave functions $\Phi(\sigma t | \sigma' t')$ and must therefore, by (5.2.2) satisfy the Schrödinger equation

$$i\hbar \frac{\partial \Phi(\sigma t | Y)}{\partial t} = \sum_{\sigma'} H_{\sigma\sigma'} \Phi(\sigma' t | Y) \quad (5.2.4)$$

where $H_{\sigma\sigma'}$ is given by (5.2.3). This establishes the Schrödinger equation for *any* spin one system in a uniform and possibly time dependent magnetic field.

5.3 Spin one particle in a non-uniform magnetic field

We now formulate the Schrödinger equation for the orbital and spinning motion of a *particle* with spin one and magnetic moment μ in a non-uniform magnetic field. Its derivation is the same as the derivation in the case of a particle of spin one-half (see section 9 of Chapter VII).

Allowing again for general external scalar and vector potentials V and \mathbf{A} to be present as well as an external magnetic field \mathbf{H} (all three of which may be any functions of position and time) we thus arrive at the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \Psi_{\sigma}}{\partial t} = \sum_{\sigma'} \left\{ H_{\sigma\sigma'} + \delta_{\sigma\sigma'} \left(-\frac{\hbar^2}{2m} \nabla^2 + V + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla + \frac{1}{2m} A^2 \right) \right\} \Psi_{\sigma'} \quad (5.3.1)$$

for any wave function $\psi_\sigma(\mathbf{r}, t)$. In (5.3.1) $H_{\sigma\sigma}$ is given by (5.2.3) in which H_x, H_y and H_z are now generally functions of position and time.

6. Spin zero systems

The nature of spin zero is covered in section 1 of Chapter VII on taking $s=0$ in that section, but again we review the specific nature of spin zero.

We may claim to know that some systems of particles (including single particle systems) are ‘spin zero systems’. They are then understood to have a spin of magnitude zero –zero, that is, over a certain time period under certain conditions or zero for all time in the case of single particles.

Spin zero is a dynamical property characterised by a dimensionless spin value s ($=0$). A spin zero system has a dimensionless ‘ z component of spin’ σ relative to a fixed Cartesian coordinate reference frame taking values $s, s-1, \dots, -s$ (i.e. 0 in any frame). At any one time and in any one such frame, σ represents a property of the system in that frame. A definite z component of spin (i.e. $\sigma=0$) in each coordinate frame of different orientation (or the same orientation occupied the other way) represents a different property. But the same z components of spin in fixed coordinate frames that differ only by a simple *translation* in space, represent the *same* property.

All propositions concerning the z components of spin in fixed Cartesian coordinate frames over a time period constitute a closed sample space S_σ . The single proposition of S_σ claiming the z component of spin σ is zero relative to a particular fixed Cartesian coordinate frame at a certain time constitutes a basis in S_σ . There is clearly no more than one natural order of such a basis, and as a result any transformation function can only equal 1, as follows from the law of unit determinate (section 3.4 of Chapter I).

Knowledge ‘ $\sigma=0$ ’ in one frame at one time (or in any number of frames at any number of times) is the only possible form of pure knowledge Y in S_σ . Since σ can have only the single value $\sigma=0$ a wave function $\Phi(\sigma|Y)$ in S_σ using the σ basis of any frame is therefore just equal to a (generally complex) number of unit modulus (i.e. equal to $e^{i\alpha}$ where α is real).

The spin/spin transformation functions $\Phi(0|0)$ (from any one coordinate frame to another at a fixed time) are therefore necessarily equal to 1. The same applies to the spin/spin transformation functions over time in one coordinate system.

The Schrödinger equation for a spin zero system therefore simply states that the rate of change of the wave function is zero. So any wave function $\Phi(\sigma|Y)$ in S_σ is constant in time and the same in all coordinate frames.

A system with spin zero may have a magnetic moment. But, on account of the spin being zero, the system’s spinning motion is not affected by a magnetic field. That is, in any one fixed Cartesian coordinate frame the values of s and σ remain zero.

VIII. Pairs of spin $\frac{1}{2}$ systems, spin 1 and spin 0

If a *particle* of spin zero carries a charge there may of course be an effect on the particle orbital motion produced by the electromagnetic potential A_{em} associated with any magnetic field. But propositions concerning the spinning motion and propositions concerning the orbital motion are logically independent because our knowledge of the particle position in space is clearly of no relevance with regard to our knowledge of its spinning motion and vice versa. Accordingly the sample space S_σ and the sample space S_r of all propositions concerning the particle's position and momentum over the same time as that covered by S_σ are logically independent, and by the law of absolute logical independence (section 3.7 of Chapter I) we can formally hold pure knowledge $Y^{(1)}$ in S_σ and pure knowledge $Y^{(2)}$ in S_r , $Y^{(1)}$ amounting simply to the proposition claiming knowledge that $s=0$ and therefore $\sigma=0$ in one or more fixed Cartesian coordinates frames. Therefore S_σ and S_r are always closed sample spaces. And the combined sample space $S_r S_\sigma$ is closed (whether or not A_{em} affects the orbital motion) and we can hold pure knowledge Y in $S_r S_\sigma$. Our wave function in $S_r S_\sigma$ can then differ from our wave function in S_r only by a constant phase factor. The Schrödinger equation for a spin zero particle is therefore the same as that (given in (4.2.4) of Chapter IV) for a particle with no spin. It does not involve the external magnetic field $\mathbf{H}(\mathbf{r}, t)$ that may be present and the wave function $\psi(\mathbf{r}, t)$ need not contain the variables s or σ because these are known to be zero at all times.

A *system* of particles known initially to have spin zero may not remain a spin zero system when it experiences a magnetic field. This is because the magnetic field will generally act differently on the spin components of the individual particles which may have different magnetic moments or be in different parts of a non-uniform magnetic field. But since the z components of spin of all particles are amenable to the principle of short time isolation, a system of spin zero will maintain its spin zero for a short time after a magnetic field is switched on. And in certain circumstances (e.g. in a uniform magnetic field with certain relations holding between the magnetic moments of the particles making up the system) the system may remain a spin zero system indefinitely.

Corresponding to the properties assumed in relation to spin one systems in section 5 we claim the following properties relating to systems known to be spin zero systems over a time period.

First property The nature of the system carrying the spin $s = 0$ and magnetic moment μ has no bearing on the value of its z component of spin in any fixed coordinate frame over the time period.

Second property When a system made up of two distinguishable spin one-half subsystems 1 and 2 with equal magnetic moments in a uniform (possibly time dependent) magnetic field, is prepared in a pure state in which its total spin is known to be zero in some time period, then (i) the system is a spin zero system in that time period, (ii) its z component of spin σ in any fixed coordinate frame is at

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any time equal to the sum of the z components of spin of the subsystems 1 and 2 in the same coordinate frame, and (iii) its magnetic moment is the sum of the magnetic moments of the subsystems 1 and 2.

The problems of finding the transformation functions $\Phi(\sigma'|\sigma)$ and $\Phi(\sigma t|\sigma' t')$ (the latter applying in a uniform (possibly time dependent) magnetic field) is (as in the case of systems of spin one in section 5) *similar* to that of finding the transformation functions $\Phi(s'\sigma'|s\sigma)$ and $\Phi(s\sigma t|s'\sigma' t')$ (with $s=s'=0$) relating to the total spin of a system made up of two subsystems of spin one-half with equal magnetic moments in the same magnetic field. And again the corresponding transformation functions (i.e. $\Phi(\sigma'|\sigma)$ and $\Phi(0\sigma'|0\sigma)$, and $\Phi(\sigma t|\sigma' t')$ and $\Phi(0\sigma t|0\sigma' t')$) are identical.

Result (3.6) thus confirms that

$$\Phi(\sigma'|\sigma) = \delta_{\sigma'\sigma} \quad \text{or} \quad \Phi(0|0) = 1,$$

and result (4.7) with (4.1.1) confirms that

$$\Phi(\sigma t|\sigma' t') = \Phi(\sigma' t'|\sigma' t') = 1 \quad \text{or} \quad \Phi(0t|0t') = 1.$$

And accordingly any wave function $\Phi(\sigma t|Y)$ for any spin zero system has the form

$$\Phi(\sigma t|Y) = \delta_{\sigma 0} e^{i\beta}$$

where the phase β remains constant.

CHAPTER IX

SPIN IN GENERAL

1. Nature of particle spin in general

The nature of particle spin in general has been covered in section 1 of Chapter VII. But we note again here that the spin of the general quantum mechanical particle is an internal physical property of the particle. It is characterised by a constant dimensionless spin value s (which has one of the possible dimensionless values $0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ depending on the particle type) and a (generally time dependent) dimensionless ‘ z component of spin’ σ relative to any one fixed Cartesian coordinate system. At any one time and relative to any one Cartesian coordinate system, σ has one of the discrete values

$$\sigma = s, s-1, \dots, -s \quad (1.1)$$

and this value is generally different in fixed coordinates with different orientations. It is a different property in each fixed Cartesian coordinate system of a different orientation or of the same orientation occupied in one or other of the two possible ways.

All propositions concerning the z components of spin in fixed Cartesian coordinate systems over a time period constitute a complete sample space S_σ . The propositions claiming one or other value of σ (relative to a particular fixed Cartesian coordinate system) is possessed by the particle at a certain time (in the time period covered by S_σ) constitute a basis in S_σ .

When a particle with non-zero spin moves in a *uniform* external magnetic field (possibly time-dependent) its spinning motion is physically independent of its orbital motion but there may be spin/field interaction (arising from a magnetic moment of the particle associated with its spin).^{*} S_σ is then *closed*. And wave functions in S_σ using a basis of the kind described above are normalised (complex-valued) probability distributions $\psi(\sigma)$.

2. The spin of a system of non-identical particles

A system composed of N non-identical particles with spins s_1, s_2, \dots, s_N has a (generally time dependent) net z component of spin σ relative to a fixed Cartesian coordinate

^{*} We suppose any quantum mechanical particle with non-zero spin has a magnetic moment, otherwise it would not be possible to claim (as we wish) that certain spin bases are primary. As we have said before, because we consider only non-relativistic theory, we may assume there is no spin/orbit interaction and no spin/spin interaction in the case of a system of particles, these processes being properly treated only in a relativistic theory.

system. And we have the following general law:

Law of spin component addition

The z component of spin σ of a system of N non-identical particles is at any time equal to the sum of the momentary z components of spin $\sigma_1, \dots, \sigma_N$ of the separate particles.

The complete sample spaces $S_{\sigma_1}, \dots, S_{\sigma_N}$ of each particle can be combined to form a complete sample space $S_{\sigma_1, \dots, \sigma_N}$ for the spinning motion of the system. And in that sample space, as the particles are non-identical, the propositions claiming possible values for each of the N components of spin $\sigma_1, \dots, \sigma_N$ relative to any one fixed Cartesian coordinate system form a basis.

But it is not always possible to form an alternative basis $s\sigma$ in $S_{\sigma_1, \dots, \sigma_N}$ where s takes on a number of possible total spin values and the system z component of spin σ takes (as in (1.1)) one of the $2s+1$ values $s, s-1, \dots, -s$ accordingly. This is evident because the law of spin component addition limits the possible values of s and prevents such a basis having the same dimension as the basis $\sigma_1, \dots, \sigma_N$. For example, for a system made up of three particles of spin $\frac{1}{2}$ the possible values of σ are $\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}$ and $-\frac{3}{2}$ allowing only s values $\frac{3}{2}$ and $\frac{1}{2}$. The dimension of a basis $s\sigma$ would therefore have to be $4+2=6$ (there being 4 values of σ going with $s = \frac{3}{2}$ and 2 values of σ going with $s = \frac{1}{2}$). But this differs from the dimension of basis $\sigma_1\sigma_2\sigma_3$ which is $2^3 = 8$.

However it *is* always possible to form an alternative basis $s\sigma$ when the system is made up of just *two* particles with spin values s_1 and s_2 . (Here s_1 may be any of the values $0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ and the same goes for s_2 . We thus have an extension of the theory we had in Chapter VII of two spin one-half particles.) We claim that the possible values of σ are then (as would follow from (1.1)) found by adding any one of the values $s_1, s_1-1, \dots, -s_1$ to any one of the values of $s_2, s_2-1, \dots, -s_2$. That is, the possible values of σ are:

$$\sigma = s_1 + s_2, s_1 + s_2 - 1, \dots, -(s_1 + s_2). \quad (2.1)$$

And we claim the possible values of s are

$$s = s_1 + s_2, s_1 + s_2 - 1, \dots, s_1 - s_2 \quad (2.2)$$

(assuming $s_1 \geq s_2$). Now there are $2(s_1 + s_2) + 1$ values of σ going with $s = s_1 + s_2$, $2(s_1 + s_2 - 1) + 1$ values of σ going with $s = s_1 + s_2 - 1, \dots$ and finally $2(s_1 - s_2) + 1$ values of σ going with $s = s_1 - s_2$. The dimension of bases $s\sigma$ must therefore be the

sum of $2(s_1 + s_2) + 1, 2(s_1 + s_2 - 1) + 1, \dots, 2(s_1 - s_2) + 1$ which works out to be equal to the dimension of basis $\sigma_1 \sigma_2$, that is, equal to $(2s_1 + 1)(2s_2 + 1)$.*

3. Combination of a pair of spin systems

When we form a system of two non-identical particles with spins s_1 and s_2 we have a system which, as we have said, has at any time a net spin s (equal to one or other of the values $s = s_1 + s_2, s_1 + s_2 - 1, \dots, |s_1 - s_2|$) and in each case a net component of spin σ taking possible values $s, s - 1, \dots, -s$ in any fixed Cartesian coordinate system. Under *certain circumstances* this system remains (over time) a system with a constant net spin s and a constant magnetic moment and behaves (as far as its net spinning motion is concerned) in the same way as would a *particle* of spin s with the same magnetic moment. This can be the case, for example, if the two particles of the system have magnetic moments proportional to their spins and the magnetic field each particle experiences is at any time the same.

Given any two such *systems* with demonstratively constant net spins s_1 and s_2 (and we include the case where one of the systems might be just a single particle) we may consider these two *systems* together as forming a system, and everything said in sections 1 and 2 with regard to *particles* and systems of *particles* applies just as well to *systems* and systems of *systems*. In particular the spin s of the combined system takes the possible values

$$s = s_1 + s_2, s_1 + s_2 - 1, \dots, |s_1 - s_2| \quad (3.1)$$

and the z component of spin σ of the combined system takes the possible values

$$\sigma = s, s - 1, \dots, -s \quad (3.2)$$

depending on the value of s .

Starting with two *particles* each of spin $\frac{1}{2}$ and magnetic moment μ , we can build up a system with net spin 1 and magnetic moment 2μ . This case has been covered already in Chapter VIII where we showed how a pair of systems of spin $\frac{1}{2}$ in a uniform magnetic field can remain a spin 1 system over time. We can, it seems, extend this method indefinitely, and in the next two sections we cover the combination of a spin $\frac{1}{2}$ particle with magnetic moment μ and a spin 1 system with magnetic moment 2μ , showing how this combination can, in a uniform magnetic field, be a ‘system of spin $\frac{3}{2}$ ’ with a magnetic moment 3μ (or alternatively a ‘system of spin $\frac{1}{2}$ ’ with magnetic moment μ) and we claim this system then behaves (as far as its net spinning motion is

* Being symmetric in s_1 and s_2 this expression clearly applies whether or not $s_1 \geq s_2$.

concerned) in the same way as a particle of spin $\frac{3}{2}$ (or as a particle of spin $\frac{1}{2}$) would. In general we claim that any system of particles that has a definite spin s of any (allowed) value and demonstratively remains a ‘system of spin s ’ in a spatially uniform magnetic field behaves (as far as its net spinning motion is concerned) in the same way as would a *particle* of spin s and a certain magnetic moment, or as would the net spinning motion of any other ‘system of spin s ’ (with the same magnetic moment) made up of spinning systems in any other manner*.

Just as we claimed a first and second property in relation to spin zero systems (section 6 of Chapter VIII) and in relation to spin one systems (section 5 of Chapter VIII), we claim first and second properties in relation to systems of any spin s and magnetic moment μ as follows.

First property The nature of a ‘system of spin s ’ with magnetic moment μ has no bearing on the value of its z component of spin in any fixed Cartesian coordinate frame at any time.

Second property When a system made up of two distinguishable subsystems of spin s_1 and s_2 , with respective magnetic moments $\mu^{(1)}$ and $\mu^{(2)}$ proportional to their spins, in a uniform (possibly time dependent) magnetic field, is prepared in any way in which its total spin is expected to be s over a time period, then (i) the system is a ‘system of spin s ’, (ii) its z component of spin σ in any fixed Cartesian coordinate frame is at any time equal to the sum of the z components of spin of the two subsystems and (iii) its magnetic moment is the sum of the magnetic moments of the two subsystems.

Note that in general we will claim, in relation to the second property, that it is the *preparation* of the system, i.e. the *acquisition of knowledge* that the system has a net spin s at a particular time, that physically ensures that its total spin remains constant under specified conditions. Unlike the case in which $s_1 = \frac{1}{2}$ and $s_2 = \frac{1}{2}$, we are not able to show in general that the net spin s of two distinguishable subsystems (of spin s_1 and s_2) has a constant net spin under certain physical conditions *independently of our knowledge*. That is why we have substituted the word ‘expected’ for the word ‘known’ in the second property stated above.

* Thus for every possible spinning motion of one system of spin s (in any prescribed time varying uniform magnetic field and relative to any prescribed fixed coordinate frame) there is an identical possible motion of any other system of spin s , and the transformation functions (from one time to another or from one fixed coordinate system to another) are accordingly the same. A system of spin s can be constructed in many ways. For example a ‘system of spin $\frac{1}{2}$ ’ could be made up of a spin $\frac{1}{2}$ particle and spin 1 particle, or of a spin $\frac{3}{2}$ particle and a spin 1 system, etc.

4. The combination of a spin one-half particle and a system of spin one

4.1 Bases for the combined system

Let us label the spin one-half particle and the spin one system 1 and 2 respectively. Then relative to any one fixed Cartesian coordinate frame we have $s_1 = \frac{1}{2}$, $s_2 = 1$, $\sigma_1 = \frac{1}{2}, -\frac{1}{2}$ and $\sigma_2 = 1, 0, -1$. In the combined sample space $S_{\sigma_1\sigma_2}$ the natural order of the basis $\sigma_1\sigma_2$ is, we suppose,*

$$\sigma_1\sigma_2 = \frac{1}{2}1, \frac{1}{2}0, \frac{1}{2}-1, -\frac{1}{2}1, -\frac{1}{2}0, -\frac{1}{2}-1 \quad (4.1.1)$$

the corresponding total spin component σ values being

$$\sigma = \sigma_1 + \sigma_2 = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2} \quad (4.1.2)$$

respectively. And the possible values of net spin s being

$$s = \frac{3}{2}, \frac{1}{2}. \quad (4.1.3)$$

The natural order of the basis $s\sigma$ we take to be

$$s\sigma = \frac{3}{2}\frac{3}{2}, \frac{3}{2}\frac{1}{2}, \frac{3}{2}-\frac{1}{2}, \frac{3}{2}-\frac{3}{2}, \frac{1}{2}\frac{1}{2}, \frac{1}{2}-\frac{1}{2} \quad (4.1.4)$$

And because of the relation $\sigma = \sigma_1 + \sigma_2$ and the limits on the possible values of s and σ we have the following propositional implications:

$$\begin{aligned} s\sigma = \frac{3}{2}\frac{3}{2} \overset{0}{\Leftrightarrow} \sigma_1\sigma_2 = \frac{1}{2}1 & \quad \sigma_1\sigma_2 = \frac{1}{2}0 \Rightarrow s\sigma = \frac{3}{2}\frac{1}{2} \text{ or } \frac{1}{2}\frac{1}{2} \\ s\sigma = \frac{3}{2}\frac{1}{2} \Rightarrow \sigma_1\sigma_2 = -\frac{1}{2}1 \text{ or } \frac{1}{2}0 & \quad \sigma_1\sigma_2 = \frac{1}{2}-1 \Rightarrow s\sigma = \frac{3}{2}-\frac{1}{2} \text{ or } \frac{1}{2}-\frac{1}{2} \\ s\sigma = \frac{3}{2}-\frac{1}{2} \Rightarrow \sigma_1\sigma_2 = \frac{1}{2}-1 \text{ or } -\frac{1}{2}0 & \quad \sigma_1\sigma_2 = -\frac{1}{2}1 \Rightarrow s\sigma = \frac{3}{2}\frac{1}{2} \text{ or } \frac{1}{2}\frac{1}{2} \\ s\sigma = \frac{3}{2}-\frac{3}{2} \overset{0}{\Leftrightarrow} \sigma_1\sigma_2 = -\frac{1}{2}-1 & \quad \sigma_1\sigma_2 = -\frac{1}{2}0 \Rightarrow^\lambda s\sigma = \frac{3}{2}-\frac{1}{2} \text{ or } \frac{1}{2}-\frac{1}{2} \\ s\sigma = \frac{1}{2}\frac{1}{2} \Rightarrow \sigma_1\sigma_2 = -\frac{1}{2}1 \text{ or } \frac{1}{2}0 & \\ s\sigma = \frac{1}{2}-\frac{1}{2} \Rightarrow \sigma_1\sigma_2 = \frac{1}{2}-1 \text{ or } -\frac{1}{2}0 & \end{aligned} \quad \dots(4.1.5)$$

* This order is derived following the general rule footnoted in section 1 of Chapter VIII. We assume systems of spin $\frac{1}{2}$ come before those of spin 1 (in the natural order of *systems*) and then we develop the Kronecker product $(\frac{1}{2} - \frac{1}{2}) \otimes (1 0 - 1)$ in the usual manner without actually evaluating the elements. This gives the order in (4.1.1).

where we claim *full* equivalence in the two cases of equivalence and $\lambda \neq 0$ in the last implication. Accordingly the transformation function taking us from wave functions in the $\sigma_1\sigma_2$ basis to corresponding wave functions in the $s\sigma$ basis (relative to one and the same coordinate system) has the (matrix) form

$$\Phi(s\sigma|\sigma_1\sigma_2) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & B & 0 & A & 0 & 0 \\ 0 & 0 & C & 0 & D & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & E & 0 & F & 0 & 0 \\ 0 & 0 & H & 0 & G & 0 \end{pmatrix} \quad (4.1.6)$$

where, as usual, the order of the columns from left to right follows the order of the basis $\sigma_1\sigma_2$, and the order of the rows from top to bottom follows the order of the basis $s\sigma$. The (possibly complex) elements A, B, \dots, G are necessarily independent of the coordinate system and of any magnetic field present.*

The transformation function taking us from wave functions in the $s\sigma$ basis to corresponding wave functions in the $\sigma_1\sigma_2$ basis is accordingly

$$\Phi(\sigma_1\sigma_2|s\sigma) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & B^* & 0 & 0 & E^* & 0 \\ 0 & 0 & C^* & 0 & 0 & H^* \\ 0 & A^* & 0 & 0 & F^* & 0 \\ 0 & 0 & D^* & 0 & 0 & G^* \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (4.1.7)$$

4.2 Transformation functions for coordinate system rotations

The ($s\sigma$ basis) transformation function for a rotation of coordinates from coordinates O to coordinates O' is, by Feynman's law

$$\Phi(s'\sigma'|s\sigma) = \sum_{\sigma'_1\sigma'_2, \sigma_1\sigma_2} \Phi(s'\sigma'|\sigma'_1\sigma'_2)\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2)\Phi(\sigma_1\sigma_2|s\sigma) \quad (4.2.1)$$

where

$$\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2) = \Phi(\sigma'_1|\sigma_1)\Phi(\sigma'_2|\sigma_2) \quad (4.2.2)$$

* The reasons for this are the same as those in the case of the elements of the transformation function $\phi_\sigma(\sigma)$ for a spin $\frac{1}{2}$ system in section 3 of Chapter VII.

the system 1 and system 2 transfer functions $\Phi(\sigma'_1|\sigma_1)$ and $\Phi(\sigma'_2|\sigma_2)$ being given in matrix form by (3.5) of Chapter VII and (5.1.1) of Chapter VIII with a, b, c and d as in (5.16) of Chapter VII. Working out the product terms we obtain the following matrix*.

$$\Phi(\sigma'_1\sigma'_2|\sigma_1\sigma_2) = \begin{pmatrix} a^3 & \sqrt{2}a^2c & ac^2 & ca^2 & \sqrt{2}ac^2 & c^3 \\ \sqrt{2}a^2b & a^2d + abc & \sqrt{2}acd & \sqrt{2}abc & cad + c^2b & \sqrt{2}c^2d \\ ab^2 & \sqrt{2}abd & ad^2 & cb^2 & \sqrt{2}bcd & cd^2 \\ ba^2 & \sqrt{2}abc & bc^2 & a^2d & \sqrt{2}acd & dc^2 \\ \sqrt{2}ab^2 & adb + b^2c & \sqrt{2}bcd & \sqrt{2}abd & ad^2 + bcd & \sqrt{2}cd^2 \\ b^3 & \sqrt{2}b^2d & bd^2 & b^2d & \sqrt{2}bd^2 & d^3 \end{pmatrix} \quad (4.2.3)$$

So by (4.2.1)

$$\begin{aligned} \Phi(s'\sigma'|s\sigma) &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & B & 0 & A & 0 & 0 \\ 0 & 0 & C & 0 & D & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & E & 0 & F & 0 & 0 \\ 0 & 0 & H & 0 & G & 0 \end{pmatrix} \begin{pmatrix} a^3 & \sqrt{2}a^2c & ac^2 & ca^2 & \sqrt{2}ac^2 & c^3 \\ \sqrt{2}a^2b & a^2d + abc & \sqrt{2}acd & \sqrt{2}abc & cad + c^2b & \sqrt{2}c^2d \\ ab^2 & \sqrt{2}abd & ad^2 & cb^2 & \sqrt{2}bcd & cd^2 \\ ba^2 & \sqrt{2}abc & bc^2 & a^2d & \sqrt{2}acd & dc^2 \\ \sqrt{2}ab^2 & adb + b^2c & \sqrt{2}bcd & \sqrt{2}abd & ad^2 + bcd & \sqrt{2}cd^2 \\ b^3 & \sqrt{2}b^2d & bd^2 & b^2d & \sqrt{2}bd^2 & d^3 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & B^* & 0 & 0 & E^* & 0 \\ 0 & 0 & C^* & 0 & 0 & H^* \\ 0 & A^* & 0 & 0 & F^* & 0 \\ 0 & 0 & D^* & 0 & 0 & G^* \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & B & 0 & A & 0 & 0 \\ 0 & 0 & C & 0 & D & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & E & 0 & F & 0 & 0 \\ 0 & 0 & H & 0 & G & 0 \end{pmatrix} \begin{pmatrix} a^3 & (B^*\sqrt{2}+A^*)a^2c & (C^*+D^*\sqrt{2})ac^2 & c^3 & (E^*\sqrt{2}+F^*)ca^2 & (H^*+G^*\sqrt{2})ac^2 \\ \sqrt{2}a^2b & B^*a^2d+(B^*+A^*\sqrt{2})abc & (D^*+C^*\sqrt{2})acd+D^*bc^2 & \sqrt{2}cd^2 & (E^*+F^*\sqrt{2})abc+E^*a^2d & (H^*\sqrt{2}+G^*)acd+G^*bc^2 \\ ab^2 & B^*\sqrt{2}abd+A^*b^2c & C^*ad^2+D^*\sqrt{2}bcd & d^2c & E^*\sqrt{2}abd+F^*b^2c & H^*ad^2+G^*\sqrt{2}bcd \\ ba^2 & B^*\sqrt{2}abc+A^*a^2d & C^*bc^2+D^*\sqrt{2}acd & dc^2 & E^*\sqrt{2}abc+F^*a^2d & H^*bc^2+G^*\sqrt{2}acd \\ \sqrt{2}ab^2 & (B^*+A^*\sqrt{2})abd+B^*b^2c & (D^*+C^*\sqrt{2})bcd+D^*ad^2 & \sqrt{2}cd^2 & (E^*+F^*\sqrt{2})abd+E^*b^2c & (H^*\sqrt{2}+G^*)bcd+G^*ad^2 \\ b^3 & (B^*\sqrt{2}+A^*)b^2d & (C^*+D^*\sqrt{2})bd^2 & d^3 & (E^*\sqrt{2}+F^*)b^2d & (H^*+G^*\sqrt{2})bd^2 \end{pmatrix} \\ &\dots (4.2.4) \end{aligned}$$

Now since the value of total spin is independent of the coordinate system, elements of the matrix $\Phi(s'\sigma'|s\sigma)$ for which $s' \neq s$ must vanish. So, for example, $\Phi(\frac{3}{2} \frac{3}{2} | \frac{1}{2} \frac{1}{2}) = 0$ and by (4.2.4) this gives $(E^*\sqrt{2} + F^*)ca^2 = 0$ and therefore $F = -E\sqrt{2}$. Similarly from $\Phi(\frac{3}{2} \frac{3}{2} | \frac{1}{2} -\frac{1}{2}) = 0$ we find $H = -G\sqrt{2}$. From $\Phi(\frac{3}{2} \frac{1}{2} | \frac{1}{2} \frac{1}{2}) = 0$ we thus obtain $B = A\sqrt{2}$ and from $\Phi(\frac{3}{2} -\frac{1}{2} | \frac{1}{2} \frac{1}{2}) = 0$ we obtain $D = C\sqrt{2}$. Setting the remaining vanishing elements of $\Phi(s'\sigma'|s\sigma)$ equal to zero gives nothing new. But we have reduced the unknowns to just four, namely A, C, E and G .

The requirement for normalisation of the wave functions $\Phi(s\sigma|\sigma_1\sigma_2)$ in (4.1.6) gives $BB^* + EE^* = 1$ and $AA^* + FF^* = 1$. Substituting $B = A\sqrt{2}$ and $F = -E\sqrt{2}$ gives

* which is the Kronecker product of matrices $\Phi(\sigma'_1|\sigma_1)$ and $\Phi(\sigma'_2|\sigma_2)$, and (as in the case of the matrix (3.1) of Chapter VIII) necessarily has a determinant equal to 1.

$EE^* = \frac{1}{3}$. Similarly from $DD^* + GG^* = 1$ and $CC^* + HH^* = 1$ we obtain $GG^* = \frac{1}{3}$. And from the requirement $CC^* + DD^* = 1$ by putting $D = C\sqrt{2}$ we find $CC^* = \frac{1}{3}$. And similarly putting $B = A\sqrt{2}$ in $AA^* + BB^* = 1$ we find $AA^* = \frac{1}{3}$.

Using these results we can simplify (4.2.4) to

$$\begin{aligned} \Phi(s'\sigma'|s\sigma) = & \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2}A & 0 & A & 0 & 0 \\ 0 & 0 & C & 0 & \sqrt{2}C & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & E & 0 & -\sqrt{2}E & 0 & 0 \\ 0 & 0 & -\sqrt{2}G & 0 & G & 0 \end{pmatrix} \begin{pmatrix} a^3 & 3A^*a^2c & 3C^*ac^2 & c^3 & 0 & 0 \\ \sqrt{2}a^2b & \sqrt{2}A^*(2abc+a^2d) & \sqrt{2}C^*(2acd+bc^2) & \sqrt{2}dc^2 & E^*(a^2d-abc) & G^*(bc^2-acd) \\ ab^2 & A^*(2abd+b^2c) & C^*(ad^2+2bcd) & d^2c & \sqrt{2}E^*(abd-b^2c) & \sqrt{2}G^*(-ad^2+bcd) \\ ba^2 & A^*(2abc+a^2d) & C^*(bc^2+2acd) & dc^2 & \sqrt{2}E^*(abc-a^2d) & \sqrt{2}G^*(-bc^2+acd) \\ \sqrt{2}ab^2 & \sqrt{2}A^*(2abd+b^2c) & \sqrt{2}C^*(2bcd+ad^2) & \sqrt{2}cd^2 & E^*(-abd+b^2c) & G^*(-bcd+ad^2) \\ b^3 & 3A^*b^2d & 3C^*bd^2 & d^3 & 0 & 0 \end{pmatrix} \\ = & \begin{pmatrix} a^3 & 3A^*a^2c & 3C^*ac^2 & c^3 & 0 & 0 \\ 3Aa^2b & 2abc+a^2d & 3AC^*(2acd+bc^2) & 3Adc^2 & 0 & 0 \\ 3Cab^2 & 3CA^*(2abd+b^2c) & ad^2+2bcd & 3Cd^2c & 0 & 0 \\ b^3 & 3A^*b^2d & 3C^*bd^2 & d^3 & 0 & 0 \\ 0 & 0 & 0 & 0 & a & -3EG^*c \\ 0 & 0 & 0 & 0 & -3GE^*b & d \end{pmatrix} \\ & \dots (4.2.5) \end{aligned}$$

where we have used the fact that $ad - bc = 1$ to simplify the four bottom right elements.

We note that the requirement of phase normalisation applied to the transfer function (4.1.6) gives

$$\det[\Phi(s\sigma|\sigma_1\sigma_2)] = BCFG - BDFH - AECG + AEDH = -9ACEG = 1$$

or

$$ACEG = -\frac{1}{9} \quad (4.2.6)$$

Finally we observe that if our system (composed of a spin one-half particle and spin one system) is known to have a net spin $\frac{1}{2}$ at one moment in time*, the problem of finding the probability distributions $\Phi(\frac{1}{2}\sigma'|\frac{1}{2}\sigma)$ (i.e. the $\Phi(s'\sigma'|s\sigma)$ with $s = s' = \frac{1}{2}$) over the possible values ($\pm \frac{1}{2}$) of σ and σ' at the time in question is, by the second property in section 3, evidently *similar* to that of finding the transfer functions $\Phi(\sigma'|\sigma)$ for a spin one-half system. Therefore $\Phi(\frac{1}{2}\sigma'|\frac{1}{2}\sigma) = \Phi(\sigma'|\sigma)e^{i\alpha}$ where the phase α is independent of σ and σ' . In matrix notation this means that in (4.2.5)

* For example, if somebody had prepared our system in a pure state such that $s\sigma = \frac{1}{2}\tilde{\sigma}$ at a certain time telling us only that s was equal to $\frac{1}{2}$ leaving us guessing what value $\tilde{\sigma}$ they chose for σ .

$$\begin{pmatrix} a & -3cEG^* \\ -3bGE^* & d \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} e^{i\alpha}$$

and here α can only be zero giving

$$EG^* = -\frac{1}{3}. \quad (4.2.7)$$

To get further we need to make a comparison between our combined spin one-half and spin one system and a system made up of three spin one-half particles.

4.3 Comparison with a system composed of three spin one-half particles

Consider a system of three distinguishable particles each with spin one-half. Let us label the particles 1, 2 and 3. The particle spins s_1, s_2 and s_3 are all equal to $\frac{1}{2}$. The propositions ‘ $\sigma_1\sigma_2\sigma_3$ ’ claiming that at one time and with respect to a fixed Cartesian coordinate system O, particle 1 has a z spin component σ_1 , particle 2 has a z spin component σ_2 and particle 3 has a z spin component σ_3 , constitute a basis in the sample space $S_{\sigma_1\sigma_2\sigma_3}$ which is the combination of the sample spaces $S_{\sigma_1}, S_{\sigma_2}$ and S_{σ_3} of each particle. We suppose the discrete basis ‘ $\sigma_1\sigma_2\sigma_3$ ’ in $S_{\sigma_1\sigma_2\sigma_3}$ has the natural order*

$$\sigma_1\sigma_2\sigma_3 = \frac{1}{2}\frac{1}{2}\frac{1}{2}, \frac{1}{2}\frac{1}{2}-\frac{1}{2}, \frac{1}{2}-\frac{1}{2}\frac{1}{2}, \frac{1}{2}-\frac{1}{2}-\frac{1}{2}, -\frac{1}{2}\frac{1}{2}\frac{1}{2}, -\frac{1}{2}\frac{1}{2}-\frac{1}{2}, -\frac{1}{2}-\frac{1}{2}\frac{1}{2}, -\frac{1}{2}-\frac{1}{2}-\frac{1}{2} \quad (4.3.1)$$

and there is a property σ which is the net z component of spin related to σ_1, σ_2 and σ_3 by

$$\sigma = \sigma_1 + \sigma_2 + \sigma_3. \quad (4.3.2)$$

There is also a property s which is the net spin of the system taking the possible values

$$\begin{aligned} s &= s_1 + s_2 + s_3, \quad s_1 + s_2 + s_3 - 1, \dots \\ &= \frac{3}{2}, \frac{1}{2} \end{aligned} \quad (4.3.3)$$

and s is, like s_1, s_2 and s_3 , independent of the coordinate system.

The possible values of σ at any one time are physically determined by the value of s at that time, σ taking one of the values

* Again this order is the order of the (unevaluated) elements in the developed Kronecker product

$$\left(\frac{1}{2} - \frac{1}{2}\right) \otimes \left(\frac{1}{2} - \frac{1}{2}\right) \otimes \left(\frac{1}{2} - \frac{1}{2}\right).$$

$$\sigma = s, s-1, \dots -s. \quad (4.3.4)$$

But as we have said in section 2, there is no *basis* $s\sigma$.

Any wave function $\Phi(\sigma_1\sigma_2\sigma_3|Y)$ under pure knowledge Y takes a different form in each fixed Cartesian coordinate system with

$$\Phi(\sigma'_1\sigma'_2\sigma'_3|Y) = \sum_{\sigma_1\sigma_2\sigma_3} \Phi(\sigma'_1\sigma'_2\sigma'_3|\sigma_1\sigma_2\sigma_3)\Phi(\sigma_1\sigma_2\sigma_3|Y) \quad (4.3.5)$$

relating the wave function in O' to that in O . The transformation function $\Phi(\sigma'_1\sigma'_2\sigma'_3|\sigma_1\sigma_2\sigma_3)$ is clearly

$$\Phi(\sigma'_1\sigma'_2\sigma'_3|\sigma_1\sigma_2\sigma_3) = \Phi(\sigma'_1|\sigma_1)\Phi(\sigma'_2|\sigma_2)\Phi(\sigma'_3|\sigma_3)$$

where $\Phi(\sigma'_1|\sigma_1), \dots$ etc. are given by (3.5) of Chapter VII. In matrix form we therefore have*

$$\Phi(\sigma'_1\sigma'_2\sigma'_3|\sigma_1\sigma_2\sigma_3) = \begin{pmatrix} a^3 & a^2c & ca^2 & ac^2 & ca^2 & ac^2 & c^2a & c^3 \\ a^2b & a^2d & abc & acd & cab & cad & c^2b & c^2d \\ ba^2 & abc & da^2 & acd & cba & bc^2 & cda & dc^2 \\ ab^2 & abd & adb & ad^2 & cb^2 & cbd & cdb & cd^2 \\ ba^2 & bac & bca & bc^2 & da^2 & dac & dca & dc^2 \\ ab^2 & bad & cb^2 & bcd & dab & ad^2 & dcb & cd^2 \\ b^2a & b^2c & bda & bdc & dba & dbc & d^2a & d^2c \\ b^3 & b^2d & db^2 & bd^2 & db^2 & bd^2 & d^2b & d^3 \end{pmatrix} \quad (4.3.6)$$

A three spin $\frac{1}{2}$ system is evidently more general (has more possible configurations) than a spin $\frac{3}{2}$ system. But a three spin $\frac{1}{2}$ system may be known (under a certain conditions) to be a spin $\frac{3}{2}$ system over a time period.

We know that under the pure state of knowledge $\sigma_1\sigma_2\sigma_3 = \frac{1}{2}\frac{1}{2}\frac{1}{2}$ for which the wave function is simply

* The matrix $\Phi(\sigma'_1\sigma'_2\sigma'_3|\sigma_1\sigma_2\sigma_3)$ is the Kronecker product of the matrices $\Phi(\sigma'_1|\sigma_1), \Phi(\sigma'_2|\sigma_2)$ and $\Phi(\sigma'_3|\sigma_3)$. Since the Kronecker product is associative the determinant of the matrix $\Phi(\sigma'_1\sigma'_2\sigma'_3|\sigma_1\sigma_2\sigma_3)$ is again equal to 1. (If \mathbf{A}, \mathbf{B} and \mathbf{C} are $n \times n, p \times p$ and $q \times q$ matrices we have $|\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C}| = |\mathbf{A} \otimes (\mathbf{B} \otimes \mathbf{C})| = |\mathbf{A}|^{pq} |\mathbf{B} \otimes \mathbf{C}|^n = |\mathbf{A}|^{pq} (|\mathbf{B}|^q |\mathbf{C}|^p)^n = |\mathbf{A}|^{pq} |\mathbf{B}|^{qn} |\mathbf{C}|^{pn}$ which equals 1 when $|\mathbf{A}| = |\mathbf{B}| = |\mathbf{C}| = 1$.)

$\Phi(s\sigma'|s\sigma)\Big|_{s\sigma'=\frac{3}{2}, s\sigma=\frac{3}{2}} = \Phi(\sigma'|\sigma)\Big|_{\sigma'=\frac{1}{2}, \sigma=\frac{3}{2}}$. Finally, we claim proposition $\sigma = \frac{3}{2}$ is fully equivalent to proposition $\sigma_1\sigma_2\sigma_3 = \frac{1}{2} \frac{1}{2} \frac{1}{2}$ so that

$$\Phi(s'\sigma'|s\sigma)\Big|_{s'\sigma'=\frac{3}{2}, s\sigma=\frac{3}{2}} = \Phi(\sigma'|\sigma)\Big|_{\sigma'=\frac{1}{2}, \sigma=\frac{3}{2}} = \Phi(\sigma' = \frac{1}{2} \Big| \frac{1}{2} \frac{1}{2} \frac{1}{2}) = \sqrt{3}a^2b.$$

Similarly we have

$$\Phi(s'\sigma'|s\sigma)\Big|_{s'\sigma'=\frac{3}{2}, s\sigma=\frac{3}{2}} = \Phi(\sigma' = -\frac{1}{2} \Big| \frac{1}{2} \frac{1}{2} \frac{1}{2}) = \sqrt{3}ab^2.$$

But in the theory of section 4.2 (on the RHS of (4.2.5)) these probabilities were given by $3Aa^2b$ and $3Cab^2$ so it must be that $A = C = \frac{1}{\sqrt{3}}$ and by (4.2.6) that $EG = -\frac{1}{3}$. And since we know (by (4.2.7)) that $EG^* = -\frac{1}{3}$, it must be that G (and therefore E) are real, and since $EE^* = GG^* = \frac{1}{3}$, that $E = \pm \frac{1}{\sqrt{3}}$ while $G = \mp \frac{1}{\sqrt{3}}$.

We can establish the signs of E and G from the claim that $\lambda \neq 0$ in (4.1.5), i.e. from

$$\sigma_1\sigma_2 = -\frac{1}{2}0 \Rightarrow^\lambda s\sigma = \frac{3}{2} - \frac{1}{2} \text{ or } \frac{1}{2} - \frac{1}{2} \quad \text{with } \lambda \neq 0. \quad (4.3.9)$$

This implies G must be $-\frac{1}{\sqrt{3}}$ (and therefore E must be $\frac{1}{\sqrt{3}}$). For if G was $\frac{1}{\sqrt{3}}$, then since $D = C\sqrt{2} = \sqrt{\frac{2}{3}}$, D and G in (4.1.6) would have the same phase (namely zero) and by the sum rule (3.4.9) of Chapter 1 we would have $\Phi(s\sigma = \frac{3}{2} - \frac{1}{2} \text{ or } \frac{1}{2} - \frac{1}{2} \Big| \sigma_1\sigma_2 = -\frac{1}{2}0) = 1$ contradicting (4.3.9).

Hence we arrive at the usual forms for the transfer functions for a combination of a spin one-half particle and a spin one system, namely

$$\Phi(s\sigma|\sigma_1\sigma_2) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{2}{3}} & 0 & \sqrt{\frac{1}{3}} & 0 & 0 \\ 0 & 0 & \sqrt{\frac{1}{3}} & 0 & \sqrt{\frac{2}{3}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \sqrt{\frac{1}{3}} & 0 & -\sqrt{\frac{2}{3}} & 0 & 0 \\ 0 & 0 & \sqrt{\frac{2}{3}} & 0 & -\sqrt{\frac{1}{3}} & 0 \end{pmatrix} \quad (4.3.10)$$

and

$$\Phi(s'\sigma'|s\sigma) = \begin{pmatrix} a^3 & \sqrt{3}a^2c & \sqrt{3}ac^2 & c^3 & 0 & 0 \\ \sqrt{3}a^2b & 2abc + a^2d & 2acd + bc^2 & \sqrt{3}dc^2 & 0 & 0 \\ \sqrt{3}ab^2 & 2abd + b^2c & ad^2 + 2bcd & \sqrt{3}d^2c & 0 & 0 \\ b^3 & \sqrt{3}b^2d & \sqrt{3}bd^2 & d^3 & 0 & 0 \\ 0 & 0 & 0 & 0 & a & c \\ 0 & 0 & 0 & 0 & b & d \end{pmatrix} \quad (4.3.11)$$

where of course a, b, c and d are given, as functions of the Euler angles, in (5.16) of Chapter VII.

5. Combination of a spin one-half particle and spin one system in a uniform magnetic field

5.1 Derivation of the Schrödinger equation

In a uniform (possibly time dependent) magnetic field \mathbf{H} a wave function $\Phi(\sigma_1\sigma_2t|Y)$ over the basis $\sigma_1\sigma_2$ in $S_{\sigma_1\sigma_2}$ (with $\sigma_1\sigma_2$ taking the possible values in (4.1.1) at any time) satisfies a Schrödinger equation that can be derived in a manner similar to the way it was done for the combination of two spin one-half systems in section 4 of Chapter VIII.

With \mathbf{H} independent of time, the spin/spin transfer function from time t' to time t is given by

$$\Phi(\sigma_1\sigma_2t|\sigma'_1\sigma'_2t') = \Phi(\sigma_1t|\sigma'_1t')\Phi(\sigma_2t|\sigma'_2t') \quad (5.1.1)$$

i.e. by the product of the transfer functions for the spin one-half particle and spin one system on their own in the separately closed sample spaces S_{σ_1} and S_{σ_2} . And the first transfer function satisfies the Schrödinger equation

$$i\hbar \frac{\partial \Phi(\sigma_1t|\sigma'_1t')}{\partial t} = \sum_{\sigma'_1} H_{\sigma_1\sigma'_1}^{(1)} \Phi(\sigma'_1t|\sigma'_1t') \quad (5.1.2)$$

and the second

$$i\hbar \frac{\partial \Phi(\sigma_2t|\sigma'_2t')}{\partial t} = \sum_{\sigma'_2} H_{\sigma_2\sigma'_2}^{(2)} \Phi(\sigma'_2t|\sigma'_2t') \quad (5.1.3)$$

where by (8.2.3) and (8.2.6) of Chapter VII

$$H_{\sigma_1\sigma'_1}^{(1)} = -\mu^{(1)} \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix} \quad (5.1.4)$$

and by (5.2.2) and (5.2.3) of Chapter VIII

$$H_{\sigma_2\sigma'_2}^{(2)} = -\mu^{(2)} \begin{pmatrix} H_z & \frac{1}{\sqrt{2}}(H_x - iH_y) & 0 \\ \frac{1}{\sqrt{2}}(H_x + iH_y) & 0 & \frac{1}{\sqrt{2}}(H_x - iH_y) \\ 0 & \frac{1}{\sqrt{2}}(H_x + iH_y) & -H_z \end{pmatrix} \quad (5.1.5)$$

where $\mu^{(1)}$ and $\mu^{(2)}$ are the magnetic moments of the particle of spin one-half and the system of spin one respectively, and the usual matrix representation is employed.

It follows that the Schrödinger equation for $\Phi(\sigma_1\sigma_2t|\sigma'_1\sigma'_2t')$ is

$$i\hbar \frac{\partial \Phi(\sigma_1\sigma_2t|\sigma'_1\sigma'_2t')}{\partial t} = \sum_{\sigma''_1\sigma''_2} H_{\sigma_1\sigma_2,\sigma''_1\sigma''_2} \Phi(\sigma''_1\sigma''_2t|\sigma'_1\sigma'_2t') \quad (5.1.6)$$

where the Hamiltonian is

$$H_{\sigma_1\sigma_1,\sigma'_2\sigma'_2} = H_{\sigma_1\sigma'_1}^{(1)} \delta_{\sigma_2\sigma'_2} + \delta_{\sigma_1\sigma'_1} H_{\sigma_2\sigma'_2}^{(2)}. \quad (5.1.7)$$

This is easily confirmed by substitution of (5.1.1) and (5.1.7) into (5.1.6).

Working in the matrix notation and employing the Kronecker product we have

$$\begin{aligned} H_{\sigma_1\sigma'_1}^{(1)} \otimes \delta_{\sigma_2\sigma'_2} &= -\mu^{(1)} \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= -\mu^{(1)} \begin{pmatrix} H_z & 0 & 0 & H_x - iH_y & 0 & 0 \\ 0 & H_z & 0 & 0 & H_x - iH_y & 0 \\ 0 & 0 & H_z & 0 & 0 & H_x - iH_y \\ H_x + iH_y & 0 & 0 & -H_z & 0 & 0 \\ 0 & H_x + iH_y & 0 & 0 & -H_z & 0 \\ 0 & 0 & H_x + iH_y & 0 & 0 & -H_z \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} \delta_{\sigma_1\sigma'_1} \otimes H_{\sigma_2\sigma'_2}^{(2)} &= -\mu^{(2)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} H_z & \frac{1}{\sqrt{2}}(H_x-iH_y) & 0 \\ \frac{1}{\sqrt{2}}(H_x+iH_y) & 0 & \frac{1}{\sqrt{2}}(H_x-iH_y) \\ 0 & \frac{1}{\sqrt{2}}(H_x+iH_y) & -H_z \end{pmatrix} \\ &= -\mu^{(2)} \begin{pmatrix} H_z & \frac{1}{\sqrt{2}}(H_x-iH_y) & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}}(H_x+iH_y) & 0 & \frac{1}{\sqrt{2}}(H_x-iH_y) & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}}(H_x+iH_y) & -H_z & 0 & 0 & 0 \\ 0 & 0 & 0 & H_z & \frac{1}{\sqrt{2}}(H_x-iH_y) & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}}(H_x+iH_y) & 0 & \frac{1}{\sqrt{2}}(H_x-iH_y) \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}}(H_x+iH_y) & -H_z \end{pmatrix} \end{aligned}$$

Adding these we find

$$H_{\sigma_1\sigma_1,\sigma'_2\sigma'_2} = - \begin{pmatrix} (\mu^{(1)}+\mu^{(2)})H_z & \frac{\mu^{(2)}}{\sqrt{2}}(H_x-iH_y) & 0 & \mu^{(1)}(H_x-iH_y) & 0 & 0 \\ \frac{\mu^{(2)}}{\sqrt{2}}(H_x+iH_y) & \mu^{(1)}H_z & \frac{\mu^{(2)}}{\sqrt{2}}(H_x-iH_y) & 0 & \mu^{(1)}(H_x-iH_y) & 0 \\ 0 & \frac{\mu^{(2)}}{\sqrt{2}}(H_x+iH_y) & (\mu^{(1)}-\mu^{(2)})H_z & 0 & 0 & \mu^{(1)}(H_x-iH_y) \\ \mu^{(1)}(H_x+iH_y) & 0 & 0 & (-\mu^{(1)}+\mu^{(2)})H_z & \frac{\mu^{(2)}}{\sqrt{2}}(H_x-iH_y) & 0 \\ 0 & \mu^{(1)}(H_x+iH_y) & 0 & \frac{\mu^{(2)}}{\sqrt{2}}(H_x+iH_y) & -\mu^{(1)}H_z & \frac{\mu^{(2)}}{\sqrt{2}}(H_x-iH_y) \\ 0 & 0 & \mu^{(1)}(H_x+iH_y) & 0 & \frac{\mu^{(2)}}{\sqrt{2}}(H_x+iH_y) & -(\mu^{(1)}+\mu^{(2)})H_z \end{pmatrix} \quad (5.1.8)$$

Since any wave function $\Phi(\sigma_1\sigma_2t|Y)$ is a linear combination of the wave functions $\Phi(\sigma_1\sigma_2t|\sigma'_1\sigma'_2t')$ (which form a complete set) it follows that the Schrödinger equation for any wave function is

$$i\hbar \frac{\partial \Phi(\sigma_1\sigma_2t|Y)}{\partial t} = \sum_{\sigma'_1\sigma'_2} H_{\sigma_1\sigma_2,\sigma'_1\sigma'_2} \Phi(\sigma'_1\sigma'_2t|Y) \quad (5.1.9)$$

with $H_{\sigma_1\sigma_1,\sigma'_2\sigma'_2}$ given by (5.1.8).

Transforming to the $s\sigma$ basis using the transformation function $\Phi(s\sigma|\sigma_1\sigma_2)$ given in (4.3.10) we get the Schrödinger equation

$$i\hbar \frac{\partial \Phi(s\sigma t|Y)}{\partial t} = \sum_{s'\sigma'} H_{s\sigma,s'\sigma'} \Phi(s'\sigma' t|Y) \quad (5.1.10)$$

where

$$H_{s\sigma,s'\sigma'} = \sum_{\sigma_1\sigma_2} \sum_{\sigma'_1\sigma'_2} \Phi(s\sigma|\sigma_1\sigma_2) H_{\sigma_1\sigma_2,\sigma'_1\sigma'_2} \Phi(\sigma'_1\sigma'_2|s'\sigma') \quad (5.1.11)$$

(cf. the derivation of (4.7) and (4.8) in Chapter VIII). Using (4.3.10) and (5.1.8) and evaluating the ordinary matrix products in (5.1.11) we obtain

$$H_{s\sigma,s'\sigma'} = \begin{pmatrix} (\mu^{(1)}+\mu^{(2)})H_z & \frac{\mu^{(1)}+\mu^{(2)}}{\sqrt{3}}(H_x-iH_y) & 0 & 0 & \frac{\mu^{(2)}-2\mu^{(1)}}{\sqrt{6}}(H_x-iH_y) & 0 \\ \frac{\mu^{(1)}+\mu^{(2)}}{\sqrt{3}}(H_x+iH_y) & \frac{\mu^{(1)}+\mu^{(2)}}{3}H_z & \frac{2(\mu^{(1)}+\mu^{(2)})}{3}(H_x-iH_y) & 0 & \frac{\sqrt{2}2\mu^{(1)}-\mu^{(2)}}{3}H_z & \frac{\mu^{(2)}-2\mu^{(1)}}{3\sqrt{2}}(H_x-iH_y) \\ 0 & \frac{2(\mu^{(1)}+\mu^{(2)})}{3}(H_x+iH_y) & -\frac{\mu^{(2)}+\mu^{(1)}}{3}H_z & \frac{\mu^{(1)}+\mu^{(2)}}{\sqrt{3}}(H_x-iH_y) & \frac{2\mu^{(1)}-\mu^{(2)}}{3\sqrt{2}}(H_x+iH_y) & \frac{\sqrt{2}2\mu^{(1)}-\mu^{(2)}}{3}H_z \\ 0 & 0 & \frac{\mu^{(1)}+\mu^{(2)}}{\sqrt{3}}(H_x+iH_y) & -(\mu^{(1)}+\mu^{(2)})H_z & 0 & \frac{2\mu^{(1)}-\mu^{(2)}}{\sqrt{6}}(H_x+iH_y) \\ \frac{\mu^{(2)}-2\mu^{(1)}}{\sqrt{6}}(H_x+iH_y) & \frac{\sqrt{2}2\mu^{(1)}-\mu^{(2)}}{3}H_z & \frac{2\mu^{(1)}-\mu^{(2)}}{3\sqrt{2}}(H_x-iH_y) & 0 & \frac{2\mu^{(2)}-\mu^{(1)}}{3}H_z & \frac{2\mu^{(2)}-\mu^{(1)}}{3}(H_x-iH_y) \\ 0 & \frac{\mu^{(2)}-2\mu^{(1)}}{\sqrt{3}\sqrt{6}}(H_x+iH_y) & \frac{\sqrt{2}2\mu^{(1)}-\mu^{(2)}}{3}H_z & \frac{2\mu^{(1)}-\mu^{(2)}}{\sqrt{6}}(H_x-iH_y) & \frac{2\mu^{(2)}-\mu^{(1)}}{3}(H_x+iH_y) & \frac{\mu^{(1)}-2\mu^{(2)}}{3}H_z \end{pmatrix} \dots(5.1.12)$$

5.2 Conditions under which the system is one of spin one-half

We suppose the combination (in section 4) of the spin one-half particle and spin one system experiences a uniform, though generally time dependent, magnetic field as in section 5.1 and that the magnetic moments $\mu^{(1)}$ and $\mu^{(2)}$ are proportional to the spins, i.e.

$$\mu^{(1)} = \mu, \quad \mu^{(2)} = 2\mu. \quad (5.2.1)$$

Then the Hamiltonian $H_{s\sigma,s'\sigma'}$ in (5.1.12) simplifies to

$$H_{s\sigma,s'\sigma'} = -\mu \begin{pmatrix} 3H_z & \sqrt{3}(H_x-iH_y) & 0 & 0 & 0 & 0 \\ \sqrt{3}(H_x+iH_y) & H_z & 2(H_x-iH_y) & 0 & 0 & 0 \\ 0 & 2(H_x+iH_y) & -H_z & \sqrt{3}(H_x-iH_y) & 0 & 0 \\ 0 & 0 & \sqrt{3}(H_x+iH_y) & -3H_z & 0 & 0 \\ 0 & 0 & 0 & 0 & H_z & H_x-iH_y \\ 0 & 0 & 0 & 0 & H_x+iH_y & -H_z \end{pmatrix} \dots(5.2.2)$$

Whenever our wave function $\Phi(s\sigma t|Y)$ is at one time (say at time $t=0$) zero for s different from $\frac{1}{2}$ and is therefore (in vector form)

$$\Phi(s\sigma 0|Y) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \alpha \\ \beta \end{pmatrix} \begin{matrix} \frac{3}{2} \frac{3}{2} \\ \frac{3}{2} \frac{1}{2} \\ \frac{3}{2} \frac{-1}{2} \\ \frac{3}{2} \frac{3}{2} \\ \frac{1}{2} \frac{1}{2} \\ \frac{1}{2} \frac{-1}{2} \end{matrix}$$

where we have labelled the elements, and α and β are complex-valued probabilities satisfying $|\alpha|^2 + |\beta|^2 = 1$, it will, by (5.1.10) with (5.2.2), clearly maintain this form over time with α and β evolving in exactly the same way as the corresponding probabilities would in the Schrödinger equation (8.2.3) of Chapter VII for a system of spin one-half.

Also, at any time, on account of the form of the transformation equation (4.3.11), the values of α and β change with our choice of fixed Cartesian coordinate frame in exactly the same way as the corresponding probabilities would for a spin one-half system.

It is therefore possible to claim (as we do) that under (5.2.1) and with the system in a uniform magnetic field, the acquisition of pure knowledge Y that includes the knowledge that the system has total spin $s = \frac{1}{2}$ at one time ensures it has spin $s = \frac{1}{2}$ at any other time and ensures it is a system of spin one-half with magnetic moment μ .

5.3 Conditions under which the system is a system of spin $\frac{3}{2}$

Under the same prescribed conditions (of uniform and generally time dependent magnetic field, and relations (5.2.1) between magnetic moments) a wave function $\Phi(s\sigma t|\tilde{Y})$ initially of the form

$$\Phi(s\sigma 0|\tilde{Y}) = \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \\ 0 \\ 0 \end{pmatrix} \begin{matrix} \frac{3}{2} \frac{3}{2} \\ \frac{3}{2} \frac{1}{2} \\ \frac{3}{2} \frac{-1}{2} \\ \frac{3}{2} \frac{3}{2} \\ \frac{1}{2} \frac{1}{2} \\ \frac{1}{2} \frac{-1}{2} \end{matrix} \quad (5.3.1)$$

where $|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$, will, by (5.1.10) and (5.2.2), clearly maintain this form over time.

We claim, as part of our general knowledge G , that the acquisition of knowledge \tilde{Y} physically ensures that the total spin of the system is and remains equal to $\frac{3}{2}$, and ensures that the system is one of spin $\frac{3}{2}$. Therefore the problem of finding a wave

function $\Phi(\sigma t|Y)$ for any system of spin $\frac{3}{2}$ where Y is pure knowledge relating to the z components of the spin $\frac{3}{2}$ in any coordinate frame, is *similar* to that of finding the wave function $\Phi(s\sigma t|\tilde{Y})$ (with $s = \frac{3}{2}$) for our combined spin one-half and spin one system under knowledge \tilde{Y} which is the same knowledge Y with regard to σ but includes the knowledge that $s = \frac{3}{2}$. Hence

$$\Phi(\sigma t|Y) = \Phi(s\sigma t|\tilde{Y}) \Big|_{s=\frac{3}{2}} e^{i\varepsilon}$$

where ε is a constant phase independent of σ and t . So the wave function $\Phi(\sigma t|Y)$ for any system of spin $\frac{3}{2}$ satisfies the Schrödinger equation

$$i\hbar \frac{\partial \Phi(\sigma t|Y)}{\partial t} = \sum_{\sigma'} H_{\sigma\sigma'} \Phi(\sigma' t|Y) \quad (5.3.2)$$

where, by (5.2.2)

$$H_{\sigma\sigma'} = -3\mu \begin{pmatrix} H_z & \frac{1}{\sqrt{3}}(H_x - iH_y) & 0 & 0 \\ \frac{1}{\sqrt{3}}(H_x + iH_y) & \frac{1}{3}H_z & \frac{2}{3}(H_x - iH_y) & 0 \\ 0 & \frac{2}{3}(H_x + iH_y) & -\frac{1}{3}H_z & \frac{1}{\sqrt{3}}(H_x - iH_y) \\ 0 & 0 & \frac{1}{\sqrt{3}}(H_x + iH_y) & -H_z \end{pmatrix} \quad (5.3.3)$$

in which 3μ is, by part (iii) of the second property in section 3, the magnetic moment of the system.

We note also that, by *similarity*, the transformation function $\Phi(\sigma'| \sigma)$ for any system of spin $\frac{3}{2}$ under rotation of coordinates is

$$\Phi(\sigma'| \sigma) = \Phi(s'\sigma'|s\sigma) \Big|_{s=\frac{3}{2}} e^{i\lambda}$$

where $\Phi(s'\sigma'|s\sigma)$ is given by (4.3.11) and λ is a constant phase independent of σ and σ' , and of the Euler angles defining the rotation. With the Euler angles set equal to zero $\Phi(\sigma'| \sigma)$ and $\Phi(s'\sigma'|s\sigma) \Big|_{s=\frac{3}{2}}$ must both equal $\delta_{\sigma\sigma'}$ so that λ can only be zero. The transformation function for a system of spin $\frac{3}{2}$ under coordinate rotation is therefore given in matrix form by

$$\Phi(\sigma'|\sigma) = \begin{pmatrix} a^3 & \sqrt{3}a^2c & \sqrt{3}ac^2 & c^3 \\ \sqrt{3}a^2b & 2abc + a^2d & 2acd + bc^2 & \sqrt{3}dc^2 \\ \sqrt{3}ab^2 & 2abd + b^2c & ad^2 + 2bcd & \sqrt{3}d^2c \\ b^3 & \sqrt{3}b^2d & \sqrt{3}bd^2 & d^3 \end{pmatrix} \quad (5.3.4)$$

6. The Schrödinger equation for the spinning and orbital motion of a spin s particle

6.1 The Schrödinger equation for spinning motion in a uniform magnetic field

Proceeding in a manner similar to that employed in section 5 in the derivation of the Schrödinger equation for the spinning motion of a system of spin $\frac{3}{2}$ in a uniform magnetic field, we can (we assume) derive the Schrödinger equation for the spinning motion of a system of any spin s in a uniform magnetic field by building such a system up from pairs of systems of smaller spins with magnetic moments proportional to their spins and using the laws of complex-valued probability claiming phases of implication in physical laws are zero or not zero as needed.

When this is done for any one value of s the Schrödinger equation is always of the form

$$i\hbar \frac{\partial \Phi(\sigma t|Y)}{\partial t} = \sum_{\sigma'} H_{\sigma\sigma'} \Phi(\sigma' t|Y) \quad (6.1.1)$$

as in (5.3.2) for the case $s = \frac{3}{2}$, in (5.2.4) of Chapter VIII for the case $s = 1$, and as in (8.2.3) of Chapter VII for the case $s = \frac{1}{2}$. The Hamiltonian can in any case be written

$$H_{\sigma\sigma'} = -\mu [\sigma_{\sigma\sigma'}^x H_x + \sigma_{\sigma\sigma'}^y H_y + \sigma_{\sigma\sigma'}^z H_z] \quad (6.1.2)$$

where H_x, H_y and H_z are the components of the magnetic field \mathbf{H} and $\sigma_{\sigma\sigma'}^x, \sigma_{\sigma\sigma'}^y$ and $\sigma_{\sigma\sigma'}^z$ are the generalised $2s+1$ by $2s+1$ spin matrices, and μ is the magnetic moment of the system.

For the case $s = \frac{1}{2}$ the spin matrices are the (Pauli) matrices given in (8.2.5) of Chapter VII. For the case $s = 1$ they are readily derived from (5.2.3) of Chapter VIII to be

$$\sigma_{\sigma\sigma'}^x = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \quad \sigma_{\sigma\sigma'}^y = \begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}, \quad \sigma_{\sigma\sigma'}^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (6.1.3)$$

and for the case $s = \frac{3}{2}$ they are, by (5.3.3)

$$\sigma_{\sigma\sigma'}^x = \begin{pmatrix} 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & \frac{2}{3} & 0 \\ 0 & \frac{2}{3} & 0 & \frac{1}{\sqrt{3}} \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 \end{pmatrix}, \quad \sigma_{\sigma\sigma'}^y = \begin{pmatrix} 0 & -\frac{i}{\sqrt{3}} & 0 & 0 \\ \frac{i}{\sqrt{3}} & 0 & -\frac{2i}{3} & 0 \\ 0 & \frac{2i}{3} & 0 & -\frac{i}{\sqrt{3}} \\ 0 & 0 & \frac{i}{\sqrt{3}} & 0 \end{pmatrix}, \quad \sigma_{\sigma\sigma'}^z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

...(6.1.4)

We can introduce a vector $\hat{\sigma}$ whose Cartesian components are the matrices $s\sigma_{\sigma\sigma'}^x, s\sigma_{\sigma\sigma'}^y$ and $s\sigma_{\sigma\sigma'}^z$ which are also the matrix forms of the operators $\hat{\sigma}_x, \hat{\sigma}_y$ and $\hat{\sigma}_z$ associated with the 'x, y and z components of spin s' defined as the z components of spin in rotated coordinates (just as was done in the case of spin one-half in section 7 of Chapter VII*). We can then write the Hamiltonian for spin s as

$$H_{\sigma\sigma'} = -\frac{\mu}{s} \hat{\sigma} \cdot \mathbf{H} \quad (6.1.5)$$

in place of (6.1.2). This generalises (8.2.8) of Chapter VII.

6.2 The Schrödinger equation for spinning and orbital motion

When the particle (of spin s and magnetic moment μ) experiences a uniform magnetic field \mathbf{H} and constant scalar and vector potentials V and \mathbf{A} , the Schrödinger equation for its spinning and orbital motion is easily derived in the same way as we did in the case of $s = \frac{1}{2}$ in section 9.1 of Chapter VII. The result, for the wave function written $\psi_{\sigma}(\mathbf{r}, t)$ or ψ_{σ} , is evidently the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi_{\sigma}}{\partial t} = \sum_{\sigma'} \left\{ -\mu [\sigma_{\sigma\sigma'}^x H_x + \sigma_{\sigma\sigma'}^y H_y + \sigma_{\sigma\sigma'}^z H_z] + \delta_{\sigma\sigma'} \left(-\frac{\hbar^2}{2m} \nabla^2 + V + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla + \frac{1}{2m} A^2 \right) \right\} \psi_{\sigma'} \quad (6.2.1)$$

the same form as in (9.1.4) of Chapter VII. Here $\sigma_{\sigma\sigma'}^x, \sigma_{\sigma\sigma'}^y$ and $\sigma_{\sigma\sigma'}^z$ are the appropriate spin matrices (examples of which were given in section 6.1) and of course m is the particle mass and $\nabla \equiv \partial/\partial \mathbf{r}$.

* with the same Euler angles used to define the rotated coordinates

For the same reasons as in section 9.2 of Chapter VII (for the case $s = \frac{1}{2}$) equation (6.2.1) also holds, and is the Schrödinger equation, when \mathbf{H} , V and \mathbf{A} are any functions of position and time.

We note that (6.2.1) can be written

$$-\frac{\hbar}{i} \frac{\partial \Psi_\sigma}{\partial t} = \sum_{\sigma'} H_{\sigma\sigma'} \Psi_{\sigma'} \quad (6.2.2)$$

with

$$H_{\sigma\sigma'} = -\frac{\mu}{s} \hat{\boldsymbol{\sigma}} \cdot \mathbf{H} + \delta_{\sigma\sigma'} \left(-\frac{\hbar^2}{2m} \nabla^2 + V + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla + \frac{1}{2m} A^2 \right) \quad (6.2.3)$$

where $\hat{\boldsymbol{\sigma}}$ is the vector operator as defined in section 6.1 and s the particle spin.

In the case \mathbf{H} has only a component H_z (i.e. when H_x and H_y are everywhere zero) the spin part of the Hamiltonian $H_{\sigma\sigma'}$ in (6.2.3) simplifies to

$$-\frac{\mu}{s} \hat{\sigma}_z H_z$$

where $\hat{\sigma}_z$ is the operator for the z component of spin s which is defined by

$$\hat{\sigma}_z \Phi(\sigma|\sigma_z) = \sigma_z \Phi(\sigma|\sigma_z) \quad (6.2.4)$$

for $\sigma_z = s, s-1, \dots, -s-1$ (cf. (7.10) of Chapter VII in the case $s = \frac{1}{2}$). Since the transformation function $\Phi(\sigma|\sigma_z)$ equals $\delta_{\sigma\sigma_z}$ the operator $\hat{\sigma}_z$ in matrix form is clearly

$$\hat{\sigma}_z = \begin{pmatrix} s & 0 & 0 & \dots & 0 \\ 0 & s-1 & 0 & & \\ 0 & 0 & & & \\ \dots & & & 0 & \\ 0 & \dots & 0 & & -s-1 \end{pmatrix} \quad (6.2.5)$$

so that in (6.2.4) $\hat{\sigma}_z$ is $\sigma_z \delta_{\sigma\sigma_z}$ and in (6.2.3) $\hat{\boldsymbol{\sigma}}$ is $\sigma \delta_{\sigma\sigma'} \mathbf{k}$ (\mathbf{k} being the unit vector in the z direction).

Accordingly the Schrödinger equation when \mathbf{H} is everywhere parallel to the z axis can be written

$$-\frac{\hbar}{i} \frac{\partial \Psi_\sigma}{\partial t} = -\frac{\mu}{s} \sigma H_z \Psi_\sigma - \frac{\hbar^2}{2m} \nabla^2 \Psi_\sigma + V \Psi_\sigma + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla \Psi_\sigma + \frac{1}{2m} A^2 \Psi_\sigma \quad (6.2.6)$$

IX. *Spin in general*

so we have a separate Schrödinger equation for each σ component of the wave function, σ of course taking the values $\sigma = s, s - 1, \dots - s - 1$.

SYSTEMS CONTAINING IDENTICAL PARTICLES

1. Bases and wave functions

In complete sample spaces of propositions concerning dynamical properties of a system of particles some of which are identical, we introduce sets of propositions that form ‘improper bases’. These are formally the same as the bases in the case the particles are all non-identical.

For example, consider a system of two identical particles and the sample space S of all propositions about the orbital motions and spinning motions of the particles over a time period. In that sample space, using a fixed Cartesian coordinate system and dividing fixed space into equal infinitesimal volume elements $d^3\mathbf{r}$, we introduce the improper basis $\xi_1\xi_2$ the general proposition of which claims that at time t the particle occurring earliest in the natural order of particles has ‘coordinates’ ξ_1 i.e. occupies the volume element $d^3\mathbf{r}_1$ at \mathbf{r}_1 and has spin component σ_1 in the z direction of the fixed Cartesian frame of reference and at the same time t the other particle has ‘coordinates’ ξ_2 i.e. occupies the (generally different) volume element $d^3\mathbf{r}_2$ at \mathbf{r}_2 and has a (generally different) spin component σ_2 in the z direction. Alternatively, with respect to the same fixed coordinate system, we might employ the improper basis p_1p_2 the general proposition of which claims that at time t the particle occurring earliest in the natural order of particles has ‘coordinates’ p_1 i.e. occupies the volume element $d^3\mathbf{p}_1$ at \mathbf{p}_1 in the *momentum* space associated with the frame of reference and has spin component σ_1 in the z direction of the frame of reference and at the same time t the other particle has ‘coordinates’ p_2 i.e. occupies the (generally different) element $d^3\mathbf{p}_2$ at \mathbf{p}_2 in the momentum space and has a (generally different) spin component σ_2 in the z direction.*

The propositions of any improper basis are not propositions whose truth could generally be known because nature provides us with no means for determining the natural

* We are using for example ξ_1 to stand both for the coordinates of a particle *and* for the proposition that claims these coordinates are possessed by the particle. We stress that in our notation (here and elsewhere when we deal with identical particles and unless we state otherwise) the natural order of the particles is reflected in the order in which the propositions (and associated coordinates) occur in a conjunction such as $\xi_1\xi_2$, while generally different *coordinate values* are marked by a numerical suffix 1,2, ...etc. So, for example ξ_1 is not necessarily associated with the particle of the system occurring earliest in the natural order of particles, and if we write $\xi_2\xi_1$ we will mean the proposition claiming that the earliest particle (in the natural order) has coordinates ξ_2 and the other particle (occurring later in the natural order) has coordinates ξ_1 .

order of identical particles. And we may not generally claim to know the natural order either (see section 3.6 of Chapter III). Therefore an improper basis is not usually a basis in the normal sense. Nonetheless, under pure knowledge Y relating to sample space S of all propositions about the orbital motions and spinning motions of the particles over a time period we will have a calculable probability distribution over the propositions of an improper basis and one determinate at least to within a constant phase factor, and we call such a probability distribution an ‘improper wave function’ or a ‘wave function over an improper basis’. (So $\Phi(\xi_1\xi_2|Y)$ is an improper wave function in the two particle example above).

We will see that the wave functions over different improper bases are related or connected to one another through transformation functions, but, because the bases are improper, these transformation functions are not generally wave functions or probability distributions under possible states of knowledge.

Now whether the identical particles are bosons or fermions, corresponding to every improper basis there is a derived proper basis (in the same sample space) that *is* a proper basis in the usual sense (except for its size in relation to the order of the sample space -see below). The propositions of this basis are the same as those of the corresponding improper basis except that they make no claim concerning which of the identical particles has which property. So, for example, corresponding to the improper basis $\xi_1\xi_2$ described above there is a proper basis denoted $[\xi_1\xi_2]$ where

$$[\xi_1\xi_2] = \xi_1\xi_2 + \xi_2\xi_1. \quad (1.1)$$

The general proposition $[\xi_1\xi_2]$ of this basis is thus the disjunction of the propositions $\xi_1\xi_2$ and $\xi_2\xi_1$, the second of which claims the particle occurring *later* (in the natural order of particles) has the coordinates ξ_1 and the particle occurring *earlier* (in the natural order of particles) has the coordinates ξ_2 .

Wave functions over improper bases (like ordinary wave functions over proper bases) cannot be just any function of the coordinates (e.g. the position/spin coordinates or the momentum/spin coordinates). The same restrictions apply to them as apply to ordinary wave functions over proper bases. For example, they must be differentiable functions of the continuous components of the coordinates and of any continuous parameters. But in addition they must have symmetry properties (see section 2). Subject to these restrictions however wave functions over improper bases may take any form and again (to within a constant phase factor) there is a 1-1 correspondence between wave functions (over any one improper basis) and pure states of knowledge.

Note that a question arises with regard to the size of bases or the order* N of the sample space S , because the number† of propositions in the improper basis $\xi_1\xi_2$, for example, is clearly greater than the number of propositions in the derived proper basis $[\xi_1\xi_2]$. As the improper bases play the more fundamental role in the theory, we adopt the convention that N equals the number of propositions in any improper basis (such as

* This is the order before we take the limit as the number of continuous coordinate values is allowed to go to infinity.

† Again, before taking the limit as the number of continuous coordinate values goes to infinity.

$\xi_1 \xi_2$) not the number in the corresponding proper basis. And this convention extends to sample spaces whose improper bases span coordinate values of any number of particles some or all of which may be identical.

Finally we claim that the sum rule for wave functions (in section 3.11 of Chapter I) applies also to wave functions over improper bases.

2. Symmetry properties of improper wave functions under the interchange of the coordinates of identical particles.

Consider a process involving certain sets of identical and (generally interacting) particles.* Let ξ denote identical particles of one type of which there may be two (or more) present. Let η denote identical particles of another type of which there may be two (or more) present,...etc. Let ξ_1, η_5, \dots etc. denote the coordinates of position and spin for each type of particle present. So for example, ξ_1 will denote one or other volume element of space and one or other z component of spin for an ξ particle depending on the value of the variable ξ_1 and so on.

If the particles in the process had all the same relevant unchanging properties (masses, spins etc) without any two being identical, then in the ordinary way, pure knowledge of the process would be present whenever we had sufficient knowledge of the dynamical properties of the system whose particles are distinguishable and can be assigned a natural order. If, in relation to the actual process, we have the same knowledge of dynamical properties except for the knowledge of which was which of the identical particles, we still have *pure* knowledge of the *actual* process.† Such knowledge (i.e. ‘full’ knowledge of the dynamical properties at one time without knowledge of the natural order of the identical particles of each kind) is in fact the general form of pure knowledge of a process containing identical particles. Under such pure states of knowledge let the (generally time dependent) improper wave functions be denoted

$$\begin{aligned} &\Phi(\xi_1 \xi_2 \dots \eta_5 \eta_6 \dots \dots t | YG), \\ &\Phi(\xi_1 \xi_2 \dots \eta_5 \eta_6 \dots \dots t | Y'G'), \\ &\Phi(\xi_1 \xi_2 \dots \eta_5 \eta_6 \dots \dots t | Y''G''), \\ &\dots \end{aligned} \tag{2.1}$$

where the time t appears explicitly and where the variables for particles of each type are, as usual, supposed to be ordered from left to right in the way nature has ordered those

* In accordance with our non-relativistic treatment we assume the particles retain their form and number during motion.

† For example we might know (of a two electron system in free space) that at time t_0 one electron is in volume element $d^3\mathbf{r}$ with z component of spin $-\frac{1}{2}$ and the other is in volume element $d^3\mathbf{r}'$ with z component of spin $+\frac{1}{2}$, but not know or be able to claim which electron (in the natural order of electrons) occupies which volume element. This would constitute pure knowledge of the two-electron system.

particles. These wave functions amount to a list of probabilities for the propositions ‘ $\xi_1\xi_2\dots\eta_5\eta_6\dots\dots$ ’ for all values of the variables $\xi_1, \xi_2, \dots; \eta_5, \eta_6, \dots; \dots$ and for all times t , under pure states of knowledge Y, Y', Y'', \dots of dynamical properties and states of general knowledge G, G', G'', \dots which possibly differ but only in regard to the external potential fields experienced by the particles (the same set of particles in every case) and the choice of rest frame. Relating (as they do) to any one time t the propositions ‘ $\xi_1\xi_2\dots\eta_5\eta_6\dots\dots$ ’ constitute a time dependent improper basis in the sample space S for the orbital and spinning motions of the particles of the system.

To deduce the symmetry properties of the improper wave functions in (2.1) we apply the method of transformation groups. We consider a transformation in which (in all our distributions (2.1)) we change the order of two variables referring to identical particles (specifically the first two ξ variables). This means the first written variable ξ_1 now refers to the particle to which ξ_2 previously referred and the second written variable ξ_2 now refers to the particle to which ξ_1 previously referred*. The problem of finding (under the same states of knowledge $YG, Y'G', Y''G'', \dots$) the new improper wave functions

$$\begin{aligned} &\tilde{\Phi}(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|YG), \\ &\tilde{\Phi}(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|Y'G'), \\ &\tilde{\Phi}(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|Y''G''), \\ &\dots \end{aligned} \tag{2.2}$$

after this transformation is *similar* to the problem of finding the original wave functions. (This is because we have no clue as to the actual natural order of the particles so this actual order can play no part in our reasoning.) Therefore we should set our degrees of belief and our relative phases of belief in all corresponding propositions equal, i.e. we should set (as in (5.1.2) of Chapter I)[†]

$$\begin{aligned} \tilde{\Phi}(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|YG) &= \Phi(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|YG)e^{i\alpha}, \\ \tilde{\Phi}(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|Y'G') &= \Phi(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|Y'G')e^{i\alpha}, \\ &\dots \end{aligned}$$

where α is a real constant (independent of the values of the coordinates $\xi_1, \xi_2, \dots; \eta_5, \eta_6, \dots; \dots$, the time t , and the states of knowledge $YG, Y'G', Y''G'', \dots$) but possibly different had we interchanged two other ξ variables or two of the η variables ...etc.

But by the second uniqueness principle of probability assignments we should also set

* i.e. to the particle 1st in the natural order of the particles of the first type present

† The alternative expression of similarity (by conjugation) is not possible (see first footnote to section 4.2).

$$\begin{aligned}\tilde{\Phi}(\xi_1\xi_2\dots\eta_5\eta_6\dots t|YG) &= \Phi(\xi_2\xi_1\dots\eta_5\eta_6\dots t|YG), \\ \tilde{\Phi}(\xi_1\xi_2\dots\eta_5\eta_6\dots t|Y'G') &= \Phi(\xi_2\xi_1\dots\eta_5\eta_6\dots t|Y'G'), \\ \dots\end{aligned}$$

because the propositions ‘ $\xi_1\xi_2\dots\eta_5\eta_6\dots t$ ’ on the LHS and ‘ $\xi_2\xi_1\dots\eta_5\eta_6\dots t$ ’ on the RHS are fully equivalent, being propositions claiming the same physical property. So we find

$$\begin{aligned}\Phi(\xi_2\xi_1\dots\eta_5\eta_6\dots t|YG) &= \Phi(\xi_1\xi_2\dots\eta_5\eta_6\dots t|YG)e^{i\alpha}, \\ \Phi(\xi_2\xi_1\dots\eta_5\eta_6\dots t|Y'G') &= \Phi(\xi_1\xi_2\dots\eta_5\eta_6\dots t|Y'G')e^{i\alpha}, \\ \dots\end{aligned}\tag{2.3}$$

i.e. the effect of interchanging the 1st and 2nd ξ coordinate values in any of the original wave functions is to multiply by $e^{i\alpha}$ regardless of the actual values of the coordinates or of the time. Doing this twice shows that $(e^{i\alpha})^2 = 1$ or

$$e^{i\alpha} = \pm 1.$$

The effect of interchanging *any* two ξ coordinate values in the original wave functions will be to multiply them by the *same* phase factor. For interchanging say the 3rd and 5th ξ coordinate values is equivalent to the set of successive interchanges of the 3rd and 1st, 2nd and 5th, 1st and 2nd, 2nd and 5th and finally of the 3rd and 1st. So if interchanging the first and second multiplies by $e^{i\alpha}$ and if interchanging the 3rd and 5th multiplies by $e^{i\beta}$, and interchanging the 3rd and 1st and the 2nd and 5th multiply by $e^{i\delta}$ and $e^{i\gamma}$ respectively, then

$$e^{i\beta} = e^{i\delta} e^{i\gamma} e^{i\alpha} e^{i\gamma} e^{i\delta}.$$

Since $e^{i\delta}$ and $e^{i\gamma}$ are each ± 1 this gives

$$e^{i\beta} = e^{i\alpha}.$$

So *all* the improper wave functions are *symmetric* or *all* the improper wave functions are *anti-symmetric* under an interchange of *any* pair of ξ coordinate values. The same can of course be said with regard to the η coordinate values or with regard to the coordinate values relating to any particles of the same type in our set of particles.*

Exactly the same symmetry or anti-symmetry property of an improper wave function applies in another representation. This can be shown simply by including

* This finding is consistent with the principle of indifference ((5.2.1) of Chapter I) which for example leads us to set $|\Phi(\xi_2\xi_1\dots\eta_5\eta_6\dots t|Y)|^2 = |\Phi(\xi_1\xi_2\dots\eta_5\eta_6\dots t|Y)|^2$ on account of us being quite indifferent as to which of the two ξ particles occurring earliest (in the natural order of ξ particles) might have which of the coordinate values ξ_1 or ξ_2 .

improper wave functions in another representation in the list (2.1) and reordering also the variables belonging to the same two particles in the tilde wave functions in the new representation. We see, then, that the symmetry or anti-symmetry property of an (original) improper wave function with respect to the interchange of any two of the coordinates of particles of one type is independent of the representation. It is also present when in addition to the various sets of identical particles non-identical particles are included in the process; the above demonstration going through unchanged. Wave functions are then still referred to as ‘improper’ or as improper with regard to the sets of identical particles of the system.

Also, since the proof of symmetry or anti-symmetry given above does not use the fact that the states of knowledge Y, Y', Y'', \dots are pure, it also holds for probability distributions (2.1) under any states of knowledge Y, Y', Y'', \dots of the dynamical properties of the system.

3. The transformation functions connecting improper wave functions

To derive these transformation functions we introduce the following physical law.

Law of motion of identical particles

The detailed laws governing the orbital and spinning motions of a system of particles some of which are identical, though unknown to us, *are exactly the same* as the detailed laws governing a similar system of non-identical particles having the same relevant properties*.

It follows that if we have a wave function over a certain improper basis, the problem of calculating the wave function in another improper basis is *similar* to that same problem for the like process involving non-identical particles in which we start out with the same wave function (to within a constant phase factor) and the improper bases have become proper bases. This leads to the required transformation functions and the Schrödinger equation being the same as the transformation functions and Schrödinger equation in the equivalent non-identical particle case.

As an example, consider a process involving just two identical particles as in section 1, and let us suppose the particles do not interact with each other through an inter-particle potential. Suppose we have pure knowledge Y of the process which does not include actual or supposed knowledge of which particle is which in the natural order. Let our corresponding improper wave function over the position/spin coordinates at one time t be $\Phi(\xi_1 \xi_2 | YG)$ and suppose, under the same state of knowledge, we want to find the

* The non-identical particles replacing the identical ones must of course have all the same properties relevant to the process considered as the identical particles they replace. But they cannot have all the same properties whatsoever or they would remain identical. So we suppose that their orbital motions are sensitive to a kind of external potential peculiar to each but not playing a part in the process considered. These peculiar potentials could in principle be used to locate and distinguish between the particles at any time of our choosing.

improper wave function $\Phi(p_1 p_2 | YG)$ in a representation using another improper basis $p_1 p_2$ (p denoting another property pertaining perhaps to another time t' , for example, the element of momentum space occupied by a particle and the z component of spin of the particle at time t'). If the particles were *non-identical* we could (because of the 1-1 correspondence between wave functions and pure states of knowledge postulated in section 3.3 of Chapter I) still start out with essentially the same wave function – i.e. with the same probability distribution (to within a constant phase factor) over the propositions $\xi_1 \xi_2$ which would then form a proper basis. Let $\tilde{Y}\tilde{G}$ be the pure knowledge corresponding to this wave function so that we have $\Phi(\xi_1 \xi_2 | \tilde{Y}\tilde{G}) = \Phi(\xi_1 \xi_2 | YG) e^{i\beta}$ where \tilde{G} differs from G only because we know the particles are non-identical in one case and identical in the other.* In the case the particles are non-identical we have, by Feynman's law,

$$\Phi(p_1 p_2 | \tilde{Y}\tilde{G}) = \sum_{\xi_1 \xi_2} \Phi(p_1 | \xi_1) \Phi(p_2 | \xi_2) \Phi(\xi_1 \xi_2 | \tilde{Y}\tilde{G}) \quad (3.1)$$

the $\Phi(p_1 | \xi_1)$ and $\Phi(p_2 | \xi_2)$ being the transformation functions in the completely separate sample spaces of the individual particles. By the law of motion of identical particles (as stated above) the problems of finding the wave functions in the $p_1 p_2$ representation in the identical and non-identical particle cases under knowledge YG and $\tilde{Y}\tilde{G}$ respectively are *similar* and by the similarity principle ((5.1.1) of Chapter I) we have

$$\Phi(p_1 p_2 | YG) = \Phi(p_1 p_2 | \tilde{Y}\tilde{G}) e^{i\alpha} \quad (3.2)$$

where α is independent of coordinates $p_1 p_2$, and of the basis $p_1 p_2$ itself. In the case that the basis $p_1 p_2$ coincides with $\xi_1 \xi_2$ i.e. that the new basis coincides with the original basis, we have $\Phi(p_1 p_2 | YG) = \Phi(p_1 p_2 | \tilde{Y}\tilde{G}) e^{-i\beta}$ by hypothesis, so the constant α must equal $-\beta$ and (3.1) gives

$$\Phi(p_1 p_2 | Y) = \sum_{\xi_1 \xi_2} \Phi(p_1 | \xi_1) \Phi(p_2 | \xi_2) \Phi(\xi_1 \xi_2 | Y) \quad (3.3)$$

where for simplicity we have dropped the general knowledge parameter G from both sides.

* In the wave function $\Phi(\xi_1 \xi_2 | \tilde{Y}\tilde{G})$ we still take ξ_1 to be the coordinates of the particle occurring earlier in the natural order of particles. Since the particles are here non-identical they are distinguishable and, as we have claimed in section 3 of Chapter III, their natural order may be harmlessly claimed in any way we please.

Hence the transformation function connecting $\Phi(\xi_1\xi_2|Y)$ to $\Phi(p_1p_2|Y)$ is the function $\Phi(p_1|\xi_1)\Phi(p_2|\xi_2)$, the same as in the non-identical particle case where we write it as $\Phi(p_1p_2|\xi_1\xi_2)$. Note well, however, that this transformation function $\Phi(p_1p_2|\xi_1\xi_2)$ with the proposition order convention of section 1, is not itself a probability distribution or wave function under knowledge $\xi_1\xi_2$ in the identical particle case because, as we have said, nature does not provide as with the means to tell, nor generally the right to claim to know, the natural order of identical particles, so the truth of $\xi_1\xi_2$ cannot generally be established. For this reason we will (here and in similar circumstances) place a hat over the phi, i.e. write the transformation function as $\hat{\Phi}(p_1p_2|\xi_1\xi_2)$ to guard against taking it as a wave function under knowledge $\xi_1\xi_2$. Thus, for a pair of identical particles Feynman's law takes the form

$$\Phi(p_1p_2|Y) = \sum_{\xi_1\xi_2} \hat{\Phi}(p_1p_2|\xi_1\xi_2)\Phi(\xi_1\xi_2|Y) \quad (3.4)$$

where $\hat{\Phi}(p_1p_2|\xi_1\xi_2) = \Phi(p_1|\xi_1)\Phi(p_2|\xi_2)$.

The above demonstration including the result (3.4) clearly extends to cases when the particles interact with each other through an inter-particle potential. The transformation function $\hat{\Phi}(p_1p_2|\xi_1\xi_2)$ is then perhaps no longer of the simple form $\Phi(p_1|\xi_1)\Phi(p_2|\xi_2)$ but is nonetheless the same as the function $\Phi(p_1p_2|\xi_1\xi_2)$ that would apply in the case of non-identical particles interacting in the same way. The demonstration also naturally extends to cover processes involving any number of particles some of which are identical.

4. The dynamic order of fermion coordinate values and the symmetry properties of improper wave functions

4.1 The dynamic order of fermion coordinate values

Any isolated system S of particles* that includes a set of identical fermions possesses a property the like of which was not met before the advent of the quantum theory. It is the property of dynamic order of fermion coordinate values.

Let ξ stand for the coordinate of position \mathbf{r} and z component of spin σ applicable to any one of a set of identical fermions of S . Now we can imagine putting all the possible values of the ξ coordinates in a certain order. Since \mathbf{r} has continuous components x, y and z , it is not as easy to express such an order mathematically as it would be if the components of ξ were all discrete, but we suppose it can in principle be done and done in an infinite number of ways corresponding to all the possible different

* i.e. a system not in interaction with other quantum mechanical systems but possibly under the influence of externally applied fields

orders.* Under one such order of ξ values we may then write for example that $\xi_3 < \xi_6$ meaning that the coordinate value ξ_3 comes before the coordinate value ξ_6 under the order in question.

We suppose that at any time t a certain *order* of all possible ξ values represents a *property* possessed by S at that time. This property is a dynamical property (called the dynamic order of ξ coordinate values) and it may change with time. There is similarly a dynamic order of p coordinate values (of momentum p and z component of spin σ) or of the ζ coordinates values of any other basis that could be employed in connection with any single fermion of the kind in question. And if S includes sets of identical fermions of different kinds there is a different time dependent property of S represented by the dynamic order of the coordinate values of each kind of fermion.

With regard to the time evolution of any dynamic order we claim the following law.

Law of evolution of the dynamic order

Under any knowledge Y of the dynamical properties of an isolated quantum mechanical system S possibly in an external field, the dynamic order of all possible coordinate values associated with any set of identical fermions of one kind stays constant at least for short times but may change abruptly from time to time. And we can take it to be a property of S amenable to the principle of short time isolation.

We claim too the following principle of free choice:

Principle of free choice of the dynamic order of coordinate values

We can never know the (generally time dependent) dynamic order of coordinate values associated with any one set of identical fermions of S , but we may assume it (specify it) in any way we please consistent with the law of evolution of the dynamic order of coordinate values and the requirements of continuity of improper wave functions. If our choice then differs from the actual dynamic order it will not matter –no contradiction between theory and experiment will arise.

Note that there is no property represented by an order (dynamic or otherwise) of coordinate values of any one of a set of identical *bosons* of a particle system. But, as we have explained, such a property does exist in the case of identical fermions. And these facts will be of importance in connection with establishing the symmetry properties of improper wave functions (section 4.2) and the relation between proper and improper wave functions for systems of identical fermions (section 6.1).

* If we divide space up into an infinite but countable number of equal tiny volume elements $\delta^3 r_i$, forming an order of the positions r_i (of the $\delta^3 r_i$) and σ values is much easier. We can then imagine taking the limit as the volume elements tend to zero in size.

4.2 The symmetry properties of improper wave functions

We established in section 2 that in any process during which the identical particles cannot be (or simply are not) claimed to have a natural order, wave functions over improper bases must be either symmetric or anti-symmetric with respect to the interchange of the coordinates of any two identical particles.

We now employ the principle of indifference to show that the wave functions (or more generally the probability distributions over coordinates under any state of knowledge Y pure or not) must in fact be *symmetric* with regard to the interchange of the coordinates of any two identical *bosons* and *anti-symmetric* with regard to the interchange of the coordinates of any two identical *fermions*.

Consider a time dependent improper wave function (or general time dependent probability distribution) $\Phi(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|Y)$ where we suppose the ξ coordinates refer to a set of identical fermions and the η coordinates refer to a set of identical bosons. (And there may also be (unwritten) coordinates referring to other sets of identical particles and to particles not identical to each other.) As previously, the order of the coordinates $\xi_1\xi_2\dots\eta_5\eta_6\dots\dots$ as written in the wave function (or probability distribution) is supposed to correspond to the natural order of the particles.

Now because we have no idea which boson comes before which in the natural order of identical η bosons we are indifferent between the propositions $\xi_1\xi_2\dots\eta_5\eta_6\dots\dots$ and $\xi_1\xi_2\dots\eta_6\eta_5\dots\dots$. Also we cannot demonstrate an absolute difference between the physical properties claimed by these propositions. Therefore we are *absolutely* indifferent between the propositions and must (by (5.2.2) of Chapter I) assign equal probabilities to them. So

$$\Phi(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|Y) = \Phi(\xi_1\xi_2\dots\eta_6\eta_5\dots\dots t|Y)$$

and it clearly follows that the wave function (or probability distribution) must be symmetric with respect to the interchange of the coordinates of any two identical bosons.* And this is true regardless of the coordinate bases employed and regardless of our knowledge Y .

Similarly, because we have no idea which fermion comes before which in the natural order of identical ξ fermions we are indifferent between the propositions $\xi_1\xi_2\dots\eta_5\eta_6\dots\dots$ and $\xi_2\xi_1\dots\eta_5\eta_6\dots\dots$. But this time, whenever $\xi_1 \neq \xi_2$, we *can* demonstrate an absolute difference between the physical properties claimed by these propositions. This is because, at time t we know there is a certain dynamic order of the

* Hence $\Phi(\xi_1\xi_2\dots\eta_5\eta_6\dots\dots t|Y) = \Phi^*(\xi_1\xi_2\dots\eta_6\eta_5\dots\dots t|Y)$ cannot be the expression of *similarity* with regard to the interchange $\eta_5 \leftrightarrow \eta_6$. And since we may claim *similarity* under interchange $\xi_1 \leftrightarrow \xi_2$ and $\eta_5 \leftrightarrow \eta_6$ together this *similarity* too (and *similarity* under the like reordering of any number of variable pairs) can only be expressed as in section 2. (See second footnote to section 8.1 of Chapter I.)

ξ coordinate values (i.e. $\xi_1 < \xi_2$ or $\xi_2 < \xi_1$) so the propositions $\xi_1\xi_2\dots\xi_5\xi_6\dots\dots$ and $\xi_2\xi_1\dots\xi_5\xi_6\dots\dots$ can, under our general knowledge G alone, be distinguished absolutely by the fact that in one case the natural order of the fermions coincides with the dynamic order of the coordinates of those particles and in the other case it does not. So for some states of knowledge Y the probabilities $\Phi(\xi_1\xi_2\dots\xi_5\xi_6\dots\dots|Y)$ and $\Phi(\xi_2\xi_1\dots\xi_5\xi_6\dots\dots|Y)$ differ with regard to their phase (see the final part of the principle of indifference section 5.2 of Chapter I). Since $\Phi(\xi_1\xi_2\dots\xi_5\xi_6\dots\dots|Y)$ must be either always symmetric or always anti-symmetric under the interchange of ξ_1 and ξ_2 , it must be anti-symmetric and it clearly follows that the wave function (or probability distribution) $\Phi(\xi_1\xi_2\dots\xi_5\xi_6\dots\dots|Y)$ must be anti-symmetric with respect to the interchange of the coordinates of any two identical fermions. And this too is true regardless of the ξ, η, \dots etc. bases employed and regardless of our knowledge Y . *

5. Processes involving non-interacting identical bosons

5.1 The relation between proper wave functions and improper wave functions

Let $\Phi(\eta_1\dots\eta_N|Y)$ be our wave function under pure knowledge Y of any process involving N identical and indistinguishable non-interacting bosons using any improper basis $\eta_1\dots\eta_N$ referring to time t .[†] We know this wave function is symmetric under the interchange of any pair of its variables and we can relate it to the wave function $\Phi([\eta_1\dots\eta_N]|Y)$ in the corresponding proper basis as follows.

The probability $\Phi([\eta_1\dots\eta_N]|Y)$ for any particular values of the variables η_1, \dots, η_N is given by the sum rule (3.11.6) of Chapter I (which as we have said applies also to improper wave functions). This is because (by definition (as in (1.1))) the proposition $[\eta_1\dots\eta_N]$ is a disjunction of the proposition $\eta_1\dots\eta_N$ and all the distinct propositions obtained from $\eta_1\dots\eta_N$ by rearranging the order of the η_i values. And, as we have shown, all these propositions have equal probabilities. When the η coordinates are all different we have $N!$ propositions in the disjunction $[\eta_1\dots\eta_N]$, and accordingly, by the sum rule (3.11.6) of Chapter I

$$\Phi([\eta_1\dots\eta_N]|Y) = \sqrt{N!} \Phi(\eta_1\dots\eta_N|Y). \quad (5.1.1)$$

* Note that this proof of the anti-symmetry of wave functions under the interchange of identical fermion coordinates would not be possible if the dynamic order of fermion coordinates was a merely conventional one rather than a real or natural one. An *absolute* difference between the propositions $\xi_1\xi_2\dots\xi_5\xi_6\dots\dots$ and $\xi_2\xi_1\dots\xi_5\xi_6\dots\dots$ would not then be present.

[†] Although the bosons are non-interacting (i.e. not interacting through an inter-particle potential) they may of course be moving under the action of an external potential field.

If however some of the η coordinates in $[\eta_1 \dots \eta_N]$ have equal values no new proposition is obtained by interchanging those particular values. Therefore to cover all possibilities we must divide the RHS of (5.1.1) by the number of ways of arranging the equal η coordinates among themselves. We first imagine the coordinates η_1, \dots, η_N to be grouped into sets each containing equal (but different) η values. Let N_1 be the number of η coordinates sharing one particular value, N_2 be the number of η coordinates sharing another particular value, and so on. Then clearly

$$N_1 + N_2 + \dots + N_m = N \quad (5.1.2)$$

where $m \leq N$ (m being equal to N only when none of the η coordinates are equal i.e. when all the numbers N_i are equal to 1). The number of ways of arranging equal values of the η coordinates amongst themselves is the product $N_1! N_2! \dots$ of the factorials of all the N_i numbers. So in general we should replace (5.1.1) by

$$\Phi([\eta_1 \dots \eta_N] | Y) = \sqrt{\frac{N!}{N_1! N_2! \dots}} \Phi(\eta_1, \dots, \eta_N | Y) \quad (5.1.3)$$

where $N_1! N_2! \dots$ is (like $\Phi(\eta_1 \dots \eta_N | Y)$) a function of the coordinates η_1, \dots, η_N . The RHS of (5.1.3) remains (as it should) symmetric with respect to the interchange of any two of the η coordinates values.

We see that (5.1.3) is the general rule for taking us from a wave function $\Phi(\eta_1 \dots \eta_N | Y)$ over an improper basis to the wave function $\Phi([\eta_1 \dots \eta_N] | Y)$ on the corresponding proper basis $[\eta_1, \dots, \eta_N]$. To go the other way, i.e. from $\Phi([\eta_1 \dots \eta_N] | Y)$ to $\Phi(\eta_1 \dots \eta_N | Y)$, we must put

$$\Phi(\eta_1 \dots \eta_N | Y) = \sqrt{\frac{N_1! N_2! \dots}{N!}} \Phi([\eta_1 \dots \eta_N] | Y) \quad (5.1.4)$$

Now we are assuming that the wave function $\Phi(\eta_1 \dots \eta_N | Y)$ must always be a differentiable function of its continuous variables. Therefore, by (5.1.4), the wave function $\Phi([\eta_1 \dots \eta_N] | Y)$ must also be a differentiable function of its continuous variables except at a set of points of configuration space where, under an infinitesimal change in the continuous variables, some of the numbers N_1, N_2, \dots change abruptly. Outside this set of points (which is of measure zero) the N_1, N_2, \dots are all equal to 1 so the original form (5.1.1) may be said to apply to all intents and purposes. Nonetheless we maintain the more general form (5.1.4) which is certainly needed *before* the limit of vanishingly small volume elements is taken, i.e. while the η coordinates are fully discrete.

5.2 The symmetrised transformation functions for bosons

We now seek ‘symmetrised transformation functions’ denoted $\hat{\Phi}(\eta_1 \dots \eta_N | [q_1 \dots q_N])$ that may connect, through the relation

$$\Phi(\eta_1 \dots \eta_N | Y) = \sum_{\{q_1 \dots q_N\}} \hat{\Phi}(\eta_1 \dots \eta_N | [q_1 \dots q_N]) \Phi([q_1 \dots q_N] | Y), \quad (5.2.1)$$

any wave function $\Phi([q_1 \dots q_N] | Y)$ over any (derived) proper basis $[q_1 \dots q_N]$ to the corresponding wave function $\Phi(\eta_1 \dots \eta_N | Y)$ over any (improper) basis $\eta_1 \dots \eta_N$ possibly referring to a different time. In (5.2.1) the sum is conducted over all possible sets $\{q_1, \dots, q_N\}$ of q values that correspond to the different propositions of the basis $[q_1 \dots q_N]$.*

We will find that the transformation functions $\hat{\Phi}(\eta_1 \dots \eta_N | [q_1 \dots q_N])$ are symmetrised combinations of the (non-symmetrised) transformation functions $\hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N)$, any one of which is defined as

$$\hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) = \Phi(\eta_1 | q_1) \dots \Phi(\eta_N | q_N) \quad (5.2.2)$$

i.e. as the simple product of the transformation functions $\Phi(\eta_1 | q_1), \dots, \Phi(\eta_N | q_N)$ in individual sample spaces for each particle.

To find the transformation functions $\hat{\Phi}(\eta_1 \dots \eta_N | [q_1 \dots q_N])$ in (5.2.1), we start with the relation

$$\Phi(\eta_1 \dots \eta_N | Y) = \sum_{q_1 \dots q_N} \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) \Phi(q_1 \dots q_N | Y), \quad (5.2.3)$$

which follows from the theory in section 3, and substitute for $\Phi(q_1 \dots q_N | Y)$ using formula (5.1.4) applied to the q representation. This gives

$$\Phi(\eta_1 \dots \eta_N | Y) = \sum_{q_1 \dots q_N} \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) \sqrt{\frac{N_1! N_2! \dots}{N!}} \Phi([q_1 \dots q_N] | Y) \quad (5.2.4)$$

* We cannot claim that (5.2.1) follows from Feynman’s law because $\eta_1 \dots \eta_N$ is not a possible pure state of knowledge and the $\eta_1 \dots \eta_N$ do not form a proper basis. The hat on the transformation function is here employed to guard us against assuming prematurely that the transformation functions are (improper) wave functions, though this will actually turn out to be true.

where N_1, N_2, \dots are functions of the variables q_1, \dots, q_N being (for any particular values of the q_1, \dots, q_N) the numbers of members in the various subsets of $\{q_1, \dots, q_N\}$ that share common values.

Now if a summand $S(q_1, \dots, q_N)$ is symmetric with respect to the interchange of any two of the variables q_1, \dots, q_N we clearly have the relation

$$\sum_{q_1 \dots q_N} S(q_1, \dots, q_N) = \sum_{\{q_1 \dots q_N\}} \frac{N!}{N_1! N_2! \dots} S(q_1, \dots, q_N) \quad (5.2.5)$$

because to get the correct value for sum on the LHS we have to multiply the summand on the RHS by the number of distinct ways of arranging the q values amongst themselves.

To apply (5.2.5) to (5.2.4) we need first to symmetrise the summand in (5.2.4). The part $\sqrt{\frac{N_1! N_2! \dots}{N!}} \Phi([q_1 \dots q_N] | Y)$ of the summand already has the symmetry required – it stays the same under any reordering of the q_1, \dots, q_N . But $\hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N)$ does not. We therefore sum (5.2.4) over all permutations P of the η_1, \dots, η_N coordinates:

$$\sum_P \Phi(\eta_1 \dots \eta_N | Y) = \sum_P \sum_{q_1 \dots q_N} \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) \sqrt{\frac{N_1! N_2! \dots}{N!}} \Phi([q_1 \dots q_N] | Y).$$

By the symmetry of the wave function $\Phi(\eta_1 \dots \eta_N | Y)$ this merely multiplies the LHS of (5.2.4) by $N!$. So we obtain

$$N! \Phi(\eta_1 \dots \eta_N | Y) = \sum_{q_1 \dots q_N} \left[\left(\sum_P \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) \right) \sqrt{\frac{N_1! N_2! \dots}{N!}} \Phi([q_1 \dots q_N] | Y) \right]$$

where, by (5.2.2), the square bracketed summand is now symmetric. Applying (5.2.5) this becomes

$$N! \Phi(\eta_1 \dots \eta_N | Y) = \sum_{\{q_1 \dots q_N\}} \frac{N!}{N_1! N_2! \dots} \left[\left(\sum_P \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) \right) \sqrt{\frac{N_1! N_2! \dots}{N!}} \Phi([q_1 \dots q_N] | Y) \right].$$

Because of the form of the $\hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N)$ in (5.2.2), P may alternatively refer to all permutations of the q_1, \dots, q_N instead of the η_1, \dots, η_N . And we can then replace the sum over all permutations P of the q_1, \dots, q_N by a sum only over the distinguishable permutations $[P]$ provided we multiply by the number of ways of ordering the equal q_1, \dots, q_N values amongst themselves, i.e. provided we multiply by $N_1! N_2! \dots$.

Hence we obtain

$$\Phi(\eta_1 \dots \eta_N | Y) = \sum_{\{q_1 \dots q_N\}} \left(\sum_{[P]} \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) \right) \sqrt{\frac{N_1! N_2! \dots}{N!}} \Phi([q_1 \dots q_N] | Y)$$

and conclude that by defining the symmetrised transformation functions to be

$$\hat{\Phi}(\eta_1 \dots \eta_N | [q_1 \dots q_N]) = \sqrt{\frac{N_1! N_2! \dots}{N!}} \sum_{[P]} \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) \quad (5.2.6)$$

we obtain the result (5.2.1). In (5.2.6), as we have already implied, $[P]$ indicates summation over the permutations of the q_1, \dots, q_N not counting permutations of equal values amongst themselves and N_1, N_2, \dots are functions of the parameters q_1, \dots, q_N (being, for any particular values of the q_1, \dots, q_N , the numbers of members in the various subsets of $\{q_1, \dots, q_N\}$ that share common values).

5.2.1 Properties of the symmetrised transformation functions

The transformation functions given in (5.2.6) are clearly symmetric with respect to an interchange of any two of the q coordinates or of any two of the η coordinates – hence the term ‘*symmetrised* transformation functions’. As their notation (bar the hat) suggests, they are wave functions under the pure knowledge that the particles possess the q coordinates q_1, \dots, q_N though which particle has which coordinate value is unknown. This is confirmed by substituting $Y = [q'_1 \dots q'_N]$ in (5.2.1) and using the orthogonality relation for transformation functions between proper bases, i.e.

$$\Phi([q_1 \dots q_N] | [q'_1 \dots q'_N]) = \delta_{\{q_1, \dots, q_N\}, \{q'_1, \dots, q'_N\}} \quad (5.2.1.1)$$

where the delta function equals 1 when the sets $\{q_1, \dots, q_N\}$ and $\{q'_1, \dots, q'_N\}$ are the same and zero otherwise. Henceforth we can therefore omit the hat on the symmetrised transformation functions.

The symmetrised transformation functions are also orthonormal, i.e.

$$\sum_{\eta_1 \dots \eta_N} \Phi^*(\eta_1 \dots \eta_N | [q_1 \dots q_N]) \Phi(\eta_1 \dots \eta_N | [q'_1 \dots q'_N]) = \delta_{\{q_1, \dots, q_N\}, \{q'_1, \dots, q'_N\}} \quad (5.2.1.2)$$

This follows by direct substitution of (5.2.6) into (5.2.1.2). Changing the order of the summation and using the known orthonormality

$$\sum_{\eta_1 \dots \eta_N} \hat{\Phi}^*(\eta_1 \dots \eta_N | q_1 \dots q_N) \hat{\Phi}(\eta_1 \dots \eta_N | q'_1 \dots q'_N) = \delta_{q_1, q'_1} \dots \delta_{q_N, q'_N}$$

the LHS of (5.2.1.2) becomes

$$\sqrt{\frac{N_1!N_2!\dots}{N!}} \sqrt{\frac{N_1'!N_2'!\dots}{N!}} \sum_{[P]} \sum_{[P']} \delta_{q_1,q_1'} \dots \delta_{q_N,q_N'} \cdot \quad (5.2.1.3)$$

For this to be non-zero we require that the set $\{q_1, \dots, q_N\}$ be the same as the set $\{q_1', \dots, q_N'\}$ otherwise the summand in (5.2.1.3) is zero for all permutations $[P]$ and $[P']$. This confirms orthogonality of the symmetrised transformation functions.

If the set $\{q_1, \dots, q_N\}$ is the same as the set $\{q_1', \dots, q_N'\}$ and all the q values are different, then for each permutation of the q values there is only one permutation of the q' values that renders the summand in (5.2.1.3) non-zero and equal to 1. The double sum is therefore a sum of $N!$ terms each equal to 1. Also $N_1, N_2, \dots; N_1', N_2', \dots$ are all equal to 1, and as a result (5.2.1.3) is itself equal to 1.

If the set $\{q_1, \dots, q_N\}$ is the same as the set $\{q_1', \dots, q_N'\}$ and some of the q values are equal then, for each distinguishable permutation of the q values, there is still only one distinguishable permutation of the q' values that renders the summand in (5.2.1.3) non-zero and equal to 1. The double sum is therefore a sum of $N!/N_1!N_2!\dots$ terms each equal to 1, and (5.2.1.3) is itself equal to 1. This confirms normality of the symmetrised transformation functions.

The symmetrised transformation functions $\Phi(\eta_1 \dots \eta_N | [q_1 \dots q_N])$ defined in (5.2.6) are also complete. That is, any wave function $\Phi(\eta_1 \dots \eta_N | Y)$ (which must of course be symmetric with respect to the interchange of any two η values) can be expressed as a linear combination of the symmetrised transformation functions for different sets of q values. This follows because we already know that the functions $\hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N)$ (with all possible q values) are complete in the sense that any function of the η variables (symmetric or not) can be expressed as a linear combination of them. When restriction is made to symmetric functions, only the symmetric combinations of the $\hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N)$, as on the RHS of (5.2.6), are needed in the linear expansion.

5.2.2 Examples of the symmetrised transformation functions

In the case of just two bosons (5.2.6) gives

$$\Phi(\eta_1, \eta_2 | [q_1 q_2]) = \begin{cases} \sqrt{\frac{1!1!}{2!}} (\hat{\Phi}(\eta_1, \eta_2 | q_1 q_2) + \hat{\Phi}(\eta_1, \eta_2 | q_2 q_1)) & q_1 \neq q_2 \\ \sqrt{\frac{2!}{2!}} \hat{\Phi}(\eta_1, \eta_2 | q_1 q_1) & q_1 = q_2 \end{cases}$$

$$= \begin{cases} \frac{1}{\sqrt{2}} (\Phi(\eta_1 | q_1) \Phi(\eta_2 | q_2) + \Phi(\eta_1 | q_2) \Phi(\eta_2 | q_1)) & q_1 \neq q_2 \\ \Phi(\eta_1 | q_1) \Phi(\eta_2 | q_1) & q_1 = q_2 \end{cases}$$

In the case of three bosons it gives, when all three q values are unequal

$$\begin{aligned} \Phi(\eta_1, \eta_2, \eta_3 | [q_1 q_2 q_3]) &= \sqrt{\frac{1!1!1!}{3!}} (\hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_1 q_2 q_3) + \hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_1 q_3 q_2) + \hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_2 q_1 q_3) \\ &\quad + \hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_2 q_3 q_1) + \hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_3 q_1 q_2) + \hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_3 q_2 q_1)) \\ &= \frac{1}{\sqrt{6}} (\Phi(\eta_1 | q_1) \Phi(\eta_2 | q_2) \Phi(\eta_3 | q_3) + \Phi(\eta_1 | q_1) \Phi(\eta_2 | q_3) \Phi(\eta_3 | q_2) \\ &\quad + \Phi(\eta_1 | q_2) \Phi(\eta_2 | q_1) \Phi(\eta_3 | q_3) + \Phi(\eta_1 | q_2) \Phi(\eta_2 | q_3) \Phi(\eta_3 | q_1) \\ &\quad + \Phi(\eta_1 | q_3) \Phi(\eta_2 | q_1) \Phi(\eta_3 | q_2) + \Phi(\eta_1 | q_3) \Phi(\eta_2 | q_2) \Phi(\eta_3 | q_1)) \end{aligned}$$

or if just two of the three q values are equal, say q_2 and q_3 , (5.2.6) gives

$$\begin{aligned} \Phi(\eta_1, \eta_2, \eta_3 | [q_1 q_2 q_2]) &= \sqrt{\frac{1!2!}{3!}} (\hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_1 q_2 q_2) + \hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_2 q_1 q_2) + \hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_2 q_2 q_1)) \\ &= \frac{1}{\sqrt{3}} (\Phi(\eta_1 | q_1) \Phi(\eta_2 | q_2) \Phi(\eta_3 | q_2) + \Phi(\eta_1 | q_2) \Phi(\eta_2 | q_1) \Phi(\eta_3 | q_2) \\ &\quad + \Phi(\eta_1 | q_2) \Phi(\eta_2 | q_2) \Phi(\eta_3 | q_1)). \end{aligned}$$

And in the case all three q values are equal it gives

$$\Phi(\eta_1, \eta_2, \eta_3 | [q_1 q_1 q_1]) = \sqrt{\frac{3!}{3!}} \hat{\Phi}(\eta_1, \eta_2, \eta_3 | q_1 q_1 q_1) = \Phi(\eta_1 | q_1) \Phi(\eta_2 | q_1) \Phi(\eta_3 | q_1).$$

5.3 Transformation functions between proper bases

Finally we seek the transformation functions $\Phi([\eta_1 \dots \eta_N] | [q_1 \dots q_N])$ in Feynman's law

$$\Phi([\eta_1 \dots \eta_N] | Y) = \sum_{\{q_1 \dots q_N\}} \Phi([\eta_1 \dots \eta_N] | [q_1 \dots q_N]) \Phi([q_1 \dots q_N] | Y) \quad (5.3.1)$$

which we know must hold between wave functions $\Phi([q_1 \dots q_N]|Y)$ and $\Phi([\eta_1 \dots \eta_N]|Y)$ over any (proper) bases $[q_1 \dots q_N]$ and $[\eta_1 \dots \eta_N]$. Putting $Y = [q_1 \dots q_N]$ in (5.1.3) we have directly using (5.2.6) the formula

$$\Phi([\eta_1 \dots \eta_N]|[q_1 \dots q_N]) = \sqrt{\frac{N!}{N_1! N_2! \dots}} \sqrt{\frac{N'_1! N'_2! \dots}{N!}} \sum_{[P]} \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N)$$

or

$$\Phi([\eta_1 \dots \eta_N]|[q_1 \dots q_N]) = \sqrt{\frac{N'_1! N'_2! \dots}{N_1! N_2! \dots}} \sum_{[P]} \hat{\Phi}(\eta_1 \dots \eta_N | q_1 \dots q_N) \quad (5.3.2)$$

In (5.3.2) $[P]$ indicates summation over the permutations of the q_1, \dots, q_N coordinates including the original arrangement q_1, \dots, q_N but not counting permutations of equal q values amongst themselves. N'_1, N'_2, \dots are the numbers of members in the various subsets of the $\{q_1, \dots, q_N\}$ that share common values. And N_1, N_2, \dots are the numbers of members in the various subsets of $\{\eta_1, \dots, \eta_N\}$ that share common values.

5.4 The validity of the various formulae when the bosons interact

All results in sections 5.1 to 5.3 have been derived assuming the (identical) bosons do not interact with each other, though they may be moving in an external field.

However the assumption of non-interaction (i.e. of no inter-particle potentials) is not needed in the derivation of some of the results and therefore those results hold also when the bosons interact. This applies to relations (5.1.3) (or (5.1.4)) between improper wave functions and the corresponding proper wave functions. So these relations clearly hold just as well when the bosons interact.

Also, all the formulae and results of sections 5.2 and 5.3 will apply when the bosons interact provided the bases employed are restricted to bases referring to one and the same time and representing properties amenable to the principle of short time isolation (section 2.1 of Chapter III). Then (5.2.2) will still hold, allowing all results in sections 5.2 and 5.3 to be derived in exactly the same way as before.

6. Processes involving non-interacting identical fermions

6.1 The relation between proper wave functions and improper wave functions

Let $\Phi(\xi_1 \dots \xi_N|Y)$ be our wave function under pure knowledge Y of any process involving N identical and indistinguishable non-interacting fermions using any improper

basis $\xi_1 \dots \xi_N$ referring to time t .^{*} We know this wave function is anti-symmetric under the interchange of any pair of ξ coordinates so, in particular, $\Phi(\xi_1 \dots \xi_N | Y)$ is zero when any two ξ coordinates are equal. We seek the relation between $\Phi(\xi_1 \dots \xi_N | Y)$ and the wave function $\Phi([\xi_1 \dots \xi_N] | Y)$ over the proper basis $[\xi_1 \dots \xi_N]$. The latter wave function is also zero when any two ξ values are equal because then each proposition in the disjunction $[\xi_1 \dots \xi_N]$ has zero probability, and by the sum rule the disjunction itself has zero probability. So in the case two (or more) ξ values are equal we have the relation

$$\Phi(\xi_1 \dots \xi_N | Y) = \Phi([\xi_1 \dots \xi_N] | Y) = 0 \quad (6.1.1)$$

and henceforth we can restrict attention to cases in which all the coordinates ξ_1, \dots, ξ_N are different.

To relate the wave functions over the bases $\xi_1 \dots \xi_N$ and $[\xi_1 \dots \xi_N]$ when all the coordinates ξ_1, \dots, ξ_N are different, we proceed as follows.

First we note that in the wave function $\Phi(\xi_1 \dots \xi_N | Y)$, $\xi_1 \dots \xi_N$ is the proposition that (at time t) the particle occurring earliest in the natural order of particles has coordinates ξ_1 , the next ξ_2 and so on. Since it is anti-symmetric, the wave function $\Phi(\xi_1 \dots \xi_N | Y)$ can be expressed in terms of the values it takes when the ξ coordinate values are *in their momentary dynamic order*. These particular values of the wave function are denoted $\Phi(\overrightarrow{\dots \xi_i \dots} | Y)$ where the long arrow indicates that the coordinate values $\{\xi_1, \dots, \xi_N\}$ are arranged (from left to right) in their dynamic order at the time in question. To reconstruct the general wave function $\Phi(\xi_1 \dots \xi_N | Y)$ we have merely to set, for any given values of ξ_1, \dots, ξ_N ,

$$\Phi(\xi_1 \dots \xi_N | Y) = \pm \Phi(\overrightarrow{\dots \xi_i \dots} | Y) \quad (6.1.2)$$

where the set of ξ values on the RHS is the same as the set of ξ values on the LHS, the plus sign applying if an even permutation will put the $\xi_1 \dots \xi_N$ (on the LHS) in their dynamic order and the minus sign applying if an odd permutation is needed.

Now, whatever the values of $\xi_1 \dots \xi_N$ in (6.1.2) and whatever their dynamic order at the time in question, the proposition $\overrightarrow{\dots \xi_i \dots}$ is equivalent to the conjunction of the proposition $[\xi_1 \dots \xi_N]$ and the proposition O_1 which claims the (fixed but unknown) natural order of the *particles* coincides at the time in question with the dynamic order of

^{*} Although the fermions are non-interacting they may of course (as in the case of bosons in section 5) be moving under the action of an external potential field.

the ξ values they possess. Since $\overrightarrow{\dots\xi_i\dots}$ and $[\xi_1\dots\xi_N]O_1$ are proposition claiming the same physical property we claim they are *fully* equivalent, so that at any time,

$$\Phi(\overrightarrow{\dots\xi_i\dots}|Y) = \Phi([\xi_1\dots\xi_N]O_1|Y). \quad (6.1.3)$$

We now claim that the propositions $[\xi_1\dots\xi_N]$ and O_1 are logically independent under knowledge Y whatever that pure state of knowledge might be. This is because under knowledge Y , *knowledge* of O_1 (even though this is not actually possible) would seemingly in no way affect the probability of $[\xi_1\dots\xi_N]$ nor seemingly would knowledge of $[\xi_1\dots\xi_N]$ in any way affect the probability of O_1 . Thus we claim (by (2.5.2) of Chapter I) that

$$\Phi([\xi_1\dots\xi_N]O_1|Y) = \Phi([\xi_1\dots\xi_N]|Y)\Phi(O_1|Y)e^{ik} \quad (6.1.4)$$

where k is the phase characteristic of knowledge Y . And from (6.1.2) and (6.1.3) we therefore have

$$\Phi(\xi_1\dots\xi_N|Y) = \pm\Phi([\xi_1\dots\xi_N]|Y)\Phi(O_1|Y)e^{ik} \quad (6.1.5)$$

where the plus sign applies if an even permutation will put the $\xi_1\dots\xi_N$ in their dynamic order and the minus sign applies if an odd permutation is needed.

To evaluate $\Phi(O_1|Y)$ we consider the more general parameterised proposition O_i ($i=1,\dots,N!$), the case $i=1$ corresponding to proposition O_1 already introduced. The proposition O_i claims the natural order of the particles bears one or other of the $N!$ relations to the order of the coordinate values they possess at time t . Clearly we are indifferent as to which of the O_i is true. And since the claims O_i are absolutely distinguishable the principle of indifference ((5.2.1) of Chapter I) applies to the propositions O_i $i=1,\dots,N!$ under knowledge Y . So by the general formula (2.2.1.8) of Chapter I we can set

$$\Phi(O_i|Y) = \frac{1}{\sqrt{N!}} e^{i(\alpha_i-k)} \quad (6.1.6)$$

where α_i is the phase characteristic of O_i under knowledge Y .

We claim further that the problem of finding the probabilities $\Phi(O_i|Y)$ $i=1,\dots,N!$ under any one state of knowledge Y is *similar* to that of finding the probabilities $\Phi(O_i|Y')$ $i=1,\dots,N!$ under any other state of knowledge Y' . This is because, even though we may claim to know the dynamic order of the ξ values over time, any knowledge Y of the dynamical properties of the identical fermion system (even if it included knowledge

of the set of coordinates $\{\xi_1, \dots, \xi_N\}$ at one time) clearly cannot help us in our calculation of the probabilities of the O_i $i=1, \dots, N!$ on account of our total lack of knowledge regarding the natural order of the particles themselves. Therefore in accordance with the similarity relation (5.1.4) of Chapter I we can write

$$\Phi(O_i|YG)e^{ik} = \Phi(O_i|G) \quad (6.1.7)$$

where k is the phase characteristic of knowledge Y whatever that knowledge of dynamical properties of the system might be.

We claim further still, that the problem of finding the probabilities $\Phi(O_i|G)$ $i=1, \dots, N!$ is *similar* to that of finding the probabilities $\Phi(O_i|G_0)$ $i=1, \dots, N!$ where G_0 may differ from G in declaring there to be no external field acting on the system of identical fermions. We can make this claim because the property of dynamic order of coordinates is one amenable to the principle of short time isolation, so that knowledge of the external field is redundant. As a result, by (5.1.5) of Chapter I,

$$\Phi(O_i|G) = \Phi(O_i|G_0) \quad (6.1.8)$$

no matter what external fields G may claim.

We note that the probabilities $\Phi(O_i|G_0)$, with the O_i referring to time t , are independent of the origin of the time. For, shifting that origin by τ can, by similarity, only change $\Phi(O_i|G_0)$ by a phase factor $e^{i\alpha}$ where α (equal of course to zero when $\tau=0$) can only be a function of τ . And since we have no parameter of the dimensions of time available, α can only be zero.

Finally we claim that the problem of finding the probabilities $\Phi(O_i|G_0)$ with the O_i referring to time t is *similar* to that of finding the probabilities $\Phi(O_i|G_0)$ with the O_i referring to another time t' . Denoting these probabilities as $\Phi(O_i t|G_0)$ and $\Phi(O_i t'|G_0)$ we thus have

$$\Phi(O_i t|G_0) = \Phi(O_i t'|G_0)e^{i\beta}$$

where the phase β is independent of i but possibly dependent on t and t' . Because the $\Phi(O_i t|G_0)$ are independent of the origin of the time, β can only be a function of $t-t'$ (zero when $t=t'$) and since again we have no parameter of the dimensions of time available, β can only be zero.

By multiplying both sides of (6.1.6) by e^{ik} and employing (6.1.7) and (6.1.8), we thus find the α_i must be independent of the time t , as well as being independent of knowledge Y and of any external field. Thus the α_i might be characteristic only of the dynamic basis ξ (i.e. of the basis abstracted from the time). The α_i in (6.1.6) are

certainly independent of the coordinate values $\{\xi_1, \dots, \xi_N\}$. Finally we choose to write α_i as $\alpha_i^{(\xi)}$ to indicate the possible dependence of the α_i on the dynamic basis in question. We thus arrive, by (6.1.6), at the formula

$$\Phi(O_1|Y)e^{ik} = \frac{1}{\sqrt{N!}} e^{i\alpha_1^{(\xi)}} \quad (6.1.9)$$

showing $\Phi(O_1|Y)e^{ik}$ is independent of the coordinate values $\{\xi_1, \dots, \xi_N\}$, of the time t to which O_1 relates, of the knowledge Y and of any external field.

Substituting this expression for $\Phi(O_1|Y)e^{ik}$ into (6.1.5) and dropping the suffix 1 on $\alpha_1^{(\xi)}$ we obtain the relation

$$\Phi(\xi_1 \dots \xi_N | Y) = \pm \frac{e^{i\alpha^{(\xi)}}}{\sqrt{N!}} \Phi([\xi_1 \dots \xi_N] | Y) \quad (6.1.10)$$

where the plus sign applies if an even permutation will put the $\xi_1 \dots \xi_N$ in their dynamic order and the minus sign applies if an odd permutation is needed. Now with a definite dynamic order of ξ values claimed, (6.1.10) establishes a complete enough relation between the wave functions over the bases $\xi_1 \dots \xi_N$ and $[\xi_1 \dots \xi_N]$. Definite relative phases of one determine the relative phases of the other. Only the absolute phase of one or the other is left undetermined.*

Now the function $\Phi(\xi_1 \dots \xi_N | Y)$, with the z components of spin held constant, has to be a differentiable function of its continuous variables. We note however that the plus or minus sign in (6.1.10) will generally change under an infinitesimal change in the continuous variables. Hence, unlike in the case of bosons (see section 5.1), the wave function $\Phi([\xi_1 \dots \xi_N] | Y)$ will be a continuous differentiable function of its continuous variables only in special cases (as for example in (7.2.3)) below.

6.2 The transformation functions between proper bases

To obtain the form of the transformation functions $\Phi([p_1 \dots p_N] | [\xi_1 \dots \xi_N])$ connecting (through Feynman's law) wave functions over contemporary bases $[\xi_1 \dots \xi_N]$ and $[p_1 \dots p_N]$ (i.e. bases referring to the same time), we start by obtaining an expression for the improper wave functions $\Phi(\xi'_1 \dots \xi'_N | [\xi_1 \dots \xi_N])$ at that time, the prime being used

* Note that it is not possible to achieve definite relative phases if we replace the supposed *natural* (dynamic) order of ξ values with a purely *conventional* one, for the relative phases of the

$\Phi([\xi_1 \dots \xi_N] | Y)$ (for any given wave function $\Phi(\xi_1 \dots \xi_N | Y)$) would then depend on our arbitrary choice of this conventional order.

merely to distinguish the ξ values relating to the propositions of the improper basis $\xi_1 \dots \xi_N$ from those relating to the proper basis $[\xi_1 \dots \xi_N]$.

Using (6.1.10) with $Y = [\xi_1 \dots \xi_N]$ we have at once that

$$\Phi(\xi'_1 \dots \xi'_N | [\xi_1 \dots \xi_N]) = \pm \frac{e^{i\alpha^{(\xi)}}}{\sqrt{N!}} \Phi([\xi'_1 \dots \xi'_N] | [\xi_1 \dots \xi_N]) = \pm \frac{e^{i\alpha^{(\xi)}}}{\sqrt{N!}} \delta_{\{\xi'_1 \dots \xi'_N\}, \{\xi_1 \dots \xi_N\}}$$

the plus sign applying when an even permutation will put the $\xi'_1 \dots \xi'_N$ in their dynamic order and the minus sign applying when an odd permutation is required.

Now we can write

$$\delta_{\{\xi'_1 \dots \xi'_N\}, \{\xi_1 \dots \xi_N\}} = \sum_P \delta_{\xi'_1, \xi_1} \dots \delta_{\xi'_N, \xi_N}$$

where P indicates summation of the leading term $\delta_{\xi'_1, \xi_1} \dots \delta_{\xi'_N, \xi_N}$ and terms derived from it by making all possible permutations of the (all different) ξ' values. Clearly only one term in the sum can be non-zero at once and this term is equal to 1 when (and only when) the sets $\{\xi'_1, \dots, \xi'_N\}$ and $\{\xi_1, \dots, \xi_N\}$ are the same. We can thus write

$$\Phi(\xi'_1 \dots \xi'_N | [\xi_1 \dots \xi_N]) = \frac{e^{i\alpha^{(\xi)}}}{\sqrt{N!}} \sum_P (\pm) \delta_{\xi'_1, \xi_1} \dots \delta_{\xi'_N, \xi_N} \quad \xi_1 < \dots < \xi_N \quad (6.2.1)$$

where the plus sign accompanies the leading term and all terms obtained from it by even permutations P of the ξ'_1, \dots, ξ'_N , and the minus sign accompanies the terms obtained by odd permutations. Result (6.2.1) holds whether or not the ξ'_1, \dots, ξ'_N are in their dynamic order.

Carrying out the transformation to the p representation we therefore obtain

$$\begin{aligned} \Phi(p_1 \dots p_N | [\xi_1 \dots \xi_N]) &= \sum_{\xi'_1 \dots \xi'_N} \hat{\Phi}(p_1 \dots p_N | \xi'_1 \dots \xi'_N) \Phi(\xi'_1 \dots \xi'_N | [\xi_1 \dots \xi_N]) \\ &= \frac{e^{i\alpha^{(\xi)}}}{\sqrt{N!}} \sum_P (\pm) \hat{\Phi}(p_1 \dots p_N | \xi_1 \dots \xi_N) \quad \xi_1 < \dots < \xi_N \\ &\dots (6.2.2) \end{aligned}$$

P and (\pm) now referring to permutations of the ξ values. Because of the form of the $\hat{\Phi}(p_1 \dots p_N | \xi_1 \dots \xi_N)$, i.e. because

$$\hat{\Phi}(p_1 \dots p_N | \xi_1 \dots \xi_N) = \Phi(p_1 | \xi_1) \dots \Phi(p_N | \xi_N) \quad (6.2.3)$$

the P in (6.2.2) may instead indicate summation over permutations of the p_1, \dots, p_N with (\pm) again applying to even and odd permutations respectively.

Now we can obtain an expression for the transformation function $\Phi([p_1 \dots p_N] | [\xi_1 \dots \xi_N])$. We use relation (6.1.10) applied to the p representation with $Y = [\xi_1 \dots \xi_N]$, and then use (6.2.2) to give

$$\begin{aligned}
 \Phi([p_1 \dots p_N] | [\xi_1 \dots \xi_N]) &= \pm \frac{\sqrt{N!}}{e^{i\alpha^{(p)}}} \Phi(p_1 \dots p_N | [\xi_1 \dots \xi_N]) \\
 &= \pm \frac{e^{i\alpha^{(\xi)}}}{e^{i\alpha^{(p)}}} \sum_P (\pm) \hat{\Phi}(p_1 \dots p_N | \xi_1 \dots \xi_N) \quad \xi_1 < \dots < \xi_N \\
 &= \frac{e^{i\alpha^{(\xi)}}}{e^{i\alpha^{(p)}}} \sum_P (\pm) \hat{\Phi}(p_1 \dots p_N | \xi_1 \dots \xi_N) \quad \xi_1 < \dots < \xi_N, p_1 < \dots < p_N \\
 &\dots(6.2.4)
 \end{aligned}$$

6.3 The symmetrised transformation functions

In section 6.2 we derived the expression (6.2.2) for the wave function $\Phi(p_1 \dots p_N | [\xi_1 \dots \xi_N])$ in any representation p given knowledge of the ξ values in any contemporary representation ξ . And the wave functions $\Phi(p_1 \dots p_N | [\xi_1 \dots \xi_N])$ for different sets of values $\{\xi_1, \dots, \xi_N\}$ serve as ‘symmetrised transformation functions’ taking us from a proper wave function $\Phi([\xi_1 \dots \xi_N] | Y)$ in any representation ξ to the corresponding improper wave function $\Phi(p_1 \dots p_N | Y)$ in any representation p . Thus even though $p_1 \dots p_N$ may not represent a possible state of knowledge it is always true that

$$\Phi(p_1 \dots p_N | Y) = \sum_{\{\xi_1 \dots \xi_N\}} \Phi(p_1 \dots p_N | [\xi_1 \dots \xi_N]) \Phi([\xi_1 \dots \xi_N] | Y). \quad (6.3.1)$$

This is because the summand is symmetric under an interchange of any two ξ values and vanishes when two ξ values are equal, so the sum is $1/N!$ times the sum over the ξ values and, using (6.2.2) and (6.1.10) we obtain for the RHS of (6.3.1) the result

$$\frac{1}{N!} \sum_{\xi_1 \dots \xi_N} \left[\frac{e^{i\alpha^{(\xi)}}}{\sqrt{N!}} \sum_P (\pm) \hat{\Phi}(p_1 \dots p_N | \xi_1 \dots \xi_N) \frac{\sqrt{N!}}{e^{i\alpha^{(\xi)}}} \Phi(\xi_1 \dots \xi_N | Y) \right]$$

where $\xi_1 < \dots < \xi_N$ and where P is supposed to refer to permutations of the p values. This reduces to

$$\frac{1}{N!} \sum_P (\pm) \Phi(p_1 \dots p_N | Y)$$

and since this sum is over $N!$ equal terms we arrive at the LHS of (6.3.1) as required.

6.3.1 Properties of the symmetrised transformation functions

Let $[\xi_1 \dots \xi_N]$ and $[p_1 \dots p_N]$ be contemporary bases then by (6.2.2) the wave functions $\Phi(\xi_1 \dots \xi_N | [p_1 \dots p_N])$ are given by

$$\Phi(\xi_1 \dots \xi_N | [p_1 \dots p_N]) = \frac{e^{i\alpha^{(p)}}}{\sqrt{N!}} \sum_P (\pm) \hat{\Phi}(\xi_1 \dots \xi_N | p_1 \dots p_N) \quad p_1 < \dots < p_N \quad (6.3.1.1)$$

where

$$\hat{\Phi}(\xi_1 \dots \xi_N | p_1 \dots p_N) = \Phi(\xi_1 | p_1) \dots \Phi(\xi_N | p_N). \quad (6.3.1.2)$$

The $\Phi(\xi_1 \dots \xi_N | [p_1 \dots p_N])$ are symmetrised transformation functions between wave functions $\Phi(\xi_1 \dots \xi_N | Y)$ and $\Phi([p_1 \dots p_N] | Y)$ representing the same pure state of knowledge. That is,

$$\Phi(\xi_1 \dots \xi_N | Y) = \sum_{\{p_1 \dots p_N\}} \Phi(\xi_1 \dots \xi_N | [p_1 \dots p_N]) \Phi([p_1 \dots p_N] | Y)$$

always holds (cf. (6.3.1)).

The symmetrised transformation functions given by (6.3.1.1) are defined only for p coordinates all different. They are clearly symmetric with respect to an interchange of any two of the p coordinates and anti-symmetric with respect to an interchange of any two of the ξ coordinates. They are zero whenever two ξ coordinates are equal and they are improper wave functions under the pure knowledge that the particles possess the unequal p coordinates p_1, \dots, p_N though which particle has which coordinate value is unknown.

The moduli, and the relative phases of the transformation functions $\Phi(\xi_1 \dots \xi_N | [p_1 \dots p_N])$ are fully determined by (6.3.1.1). Only the absolute phase (the value of $e^{i\alpha^{(p)}}$) remains indeterminate.

The symmetrised transformation functions are orthonormal, i.e.

$$\sum_{\xi_1 \dots \xi_N} \Phi^*(\xi_1 \dots \xi_N | [p_1 \dots p_N]) \Phi(\xi_1 \dots \xi_N | [p'_1 \dots p'_N]) = \delta_{\{p_1 \dots p_N\}, \{p'_1 \dots p'_N\}} \quad (6.3.1.3)$$

This follows by substitution of (6.3.1.1) into (6.3.1.3) taking P and (\pm) to refer to the p coordinates. Changing the order of the summation and using the known orthonormality

$$\sum_{\xi_1 \dots \xi_N} \hat{\Phi}^*(\xi_1 \dots \xi_N | p_1 \dots p_N) \hat{\Phi}(\xi_1 \dots \xi_N | p'_1 \dots p'_N) = \delta_{p_1, p'_1} \dots \delta_{p_N, p'_N}$$

the LHS of (6.3.1.3) becomes

$$\frac{1}{\sqrt{N!}} \frac{1}{\sqrt{N!}} \sum_P \sum_{P'} (\pm)(\pm)' \delta_{p_1, p'_1} \dots \delta_{p_N, p'_N} \cdot \quad (6.3.1.4)$$

For this to be non-zero we require that the set $\{p_1, \dots, p_N\}$ be the same as the set $\{p'_1, \dots, p'_N\}$ otherwise the summand in (6.3.1.4) is zero for all permutations P and P' . This confirms orthogonality of the symmetrised transformation functions. If the set $\{p_1, \dots, p_N\}$ is the same as the set $\{p'_1, \dots, p'_N\}$, then for each permutation of the p values there is only one permutation of the p' values that renders the summand in (6.3.1.4) non-zero and equal to 1. The double sum is therefore a sum of $N!$ terms each equal to 1, and as a result (6.3.1.4) is itself equal to 1.

The symmetrised transformation functions $\Phi(\xi_1 \dots \xi_N | [p_1 \dots p_N])$ defined in (6.3.1.1) are also complete. That is, any wave function $\Phi(\xi_1 \dots \xi_N | Y)$ (which must of course be anti-symmetric with respect to the interchange of any two ξ coordinates) can be expressed as a linear combination of the symmetrised transformation functions for different sets of p values. This follows because we already know that the functions $\hat{\Phi}(\xi_1 \dots \xi_N | p_1 \dots p_N)$ (for any ordered p values) are complete in the sense that any function of the ξ variables (anti-symmetric or not) can be expressed as a linear combination of them. When restriction is made to anti-symmetric functions only the anti-symmetric combinations of $\hat{\Phi}(\xi_1 \dots \xi_N | p_1 \dots p_N)$, as on the RHS of (6.3.1.1), are needed in the linear expansion.

As in the case of bosons, though orthonormal and complete, the symmetrised transformation functions are not transformation functions in the usual sense because the $\xi_1 \dots \xi_N$ do not generally form a proper basis.

6.3.2 Examples of the symmetrised transformation functions

Taking by convention $e^{i\alpha^{(p)}} = 1$ in (6.3.1.1), and using (6.3.1.2), we obtain the following results.

In the case of just two fermions (6.3.1.1) gives

$$\Phi(\xi_1 \xi_2 | [p_1 p_2]) = \frac{1}{\sqrt{2!}} \left(\hat{\Phi}(\xi_1 \xi_2 | p_1 p_2) - \hat{\Phi}(\xi_2 \xi_1 | p_1 p_2) \right)$$

$$= \frac{1}{\sqrt{2}} \left(\Phi(\xi_1|p_1)\Phi(\xi_2|p_2) - \Phi(\xi_2|p_1)\Phi(\xi_1|p_2) \right), \quad p_1 < p_2. \quad (6.3.2.1)$$

In the case of three fermions (6.3.1.1) gives

$$\begin{aligned} \Phi(\xi_1\xi_2\xi_3|[p_1p_2p_3]) &= \frac{1}{\sqrt{3!}} \left(\hat{\Phi}(\xi_1\xi_2\xi_3|p_1p_2p_3) - \hat{\Phi}(\xi_2\xi_1\xi_3|p_1p_2p_3) + \hat{\Phi}(\xi_2\xi_3\xi_1|p_1p_2p_3) \right. \\ &\quad \left. - \hat{\Phi}(\xi_3\xi_2\xi_1|p_1p_2p_3) + \hat{\Phi}(\xi_3\xi_1\xi_2|p_1p_2p_3) - \hat{\Phi}(\xi_1\xi_3\xi_2|p_1p_2p_3) \right) \\ &= \frac{1}{\sqrt{6}} \left(\Phi(\xi_1|p_1)\Phi(\xi_2|p_2)\Phi(\xi_3|p_3) - \Phi(\xi_2|p_1)\Phi(\xi_1|p_2)\Phi(\xi_3|p_3) \right. \\ &\quad \left. + \Phi(\xi_2|p_1)\Phi(\xi_3|p_2)\Phi(\xi_1|p_3) - \Phi(\xi_3|p_1)\Phi(\xi_2|p_2)\Phi(\xi_1|p_3) \right. \\ &\quad \left. + \Phi(\xi_3|p_1)\Phi(\xi_1|p_2)\Phi(\xi_2|p_3) - \Phi(\xi_1|p_1)\Phi(\xi_3|p_2)\Phi(\xi_2|p_3) \right), \\ &\quad p_1 < p_2 < p_3. \quad (6.3.2.2) \end{aligned}$$

6.4 The validity of the various formulae when the fermions interact

As in the case of systems of identical bosons, results of sections 6.1 to 6.3 may hold also when the identical fermions interact.

The arguments leading for example to the momentary relation (6.1.10) between the improper and proper wave functions are quite independent of whether or not the particles interact. So (6.1.10) still holds when they are in interaction.

Also the arguments leading to the transformation functions between proper bases (section 6.2) and to the symmetrised transformation functions (section 6.3) are valid when the particles interact provided the ξ and p bases refer to the same time and represent properties amenable to the principle of short time isolation. For then equation (6.2.3) on which the arguments depend will still be true.

7. Wave functions for distinguishable and non-interacting identical particles

We have said before that identical particles can sometimes have distinctive properties that enable us to distinguish between them and gain knowledge of which is which at any time during their motion. (See section 3.5 of Chapter III.) If, for example, two identical non-interacting particles* are well separated in space, we are able to distinguish between them on account of this separation, and to have pure states of knowledge of each. If the state of complete separation is maintained over a time period our separate pure knowledge of each is also maintained. The question then arises as to how our wave function for the pair (which is the product of a function of the coordinates of one and a function of the

* Although the particles are non-interacting they may of course be moving under the action of an external potential.

coordinates of the other) is related to the wave functions over the proper or improper bases employed so far.

7.1 Case of identical bosons

Suppose, for example the particles are identical *bosons*, and one of them (we call particle A) is known to be within a (generally moving) region A and the other (we call particle B) within a (generally moving) region B always well separated from A. Under pure knowledge Y and in sample spaces of the kind $S_{\sigma r}$ of section 2.3 of Chapter III we may have wave functions $\Phi_A(\eta_A|Y)$ and $\Phi_B(\eta_B|Y)$ (moving wave packets confined to moving regions A and B respectively*) η_A and η_B being coordinates denoting a general volume element of space and z component of spin for particles A and B respectively. Since the particles are distinguishable and non-interacting the sample spaces $S_{\sigma r}^A$ and $S_{\sigma r}^B$ for each are closed, and for the purposes of argument we suppose they are both confined to propositions referring to any one time t only. Our wave function over the proper basis $\eta_A\eta_B$ in the sample space S that is the combination $S_{\sigma r}^A S_{\sigma r}^B$ of the sample spaces for each particle is, by (2.2) of Chapter II

$$\Phi(\eta_A\eta_B|Y) = \Phi_A(\eta_A|Y)\Phi_B(\eta_B|Y)e^{ik} \quad (7.1.1)$$

where k is the phase characteristic of knowledge Y .

But under the same pure knowledge Y and making no claim with regard to the natural order of the particles, we expect there is (in the same sample space S) an improper wave function $\Phi(\eta_1\eta_2|Y)$ expressing the probability that the particle occurring earliest (in the natural order of particles) has coordinates η_1 and the other has coordinates η_2 . The question now arises as to what is the relation between $\Phi(\eta_1\eta_2|Y)$ and $\Phi_A(\eta_A|Y)\Phi_B(\eta_B|Y)$.

To find it by logical deduction we may reasonably argue that the proposition $[\eta_1\eta_2]$ (claiming the particle occurring *earlier* in the natural order of particles has coordinates η_1 and the other η_2 -or- the particle occurring *later* in the natural order of particles has coordinates η_1 and the other η_2) is *fully equivalent* to the proposition $\eta_A\eta_B$ (of the basis $\eta_A\eta_B$ in S) when

$$(\eta_1 = \eta_A \text{ and } \eta_2 = \eta_B) \text{ or } (\eta_1 = \eta_B \text{ and } \eta_2 = \eta_A).$$

* Of course the wave packets cannot remain *totally* non-overlapping over time, but we assume throughout section 7 (and elsewhere) that the degree of overlap of 'well separates particles' over the time periods considered is so weak as to be unimportant.

That is, under this relation $[\eta_1\eta_2] \overset{0}{\leftrightarrow} \eta_A\eta_B$, and the probability of $[\eta_1\eta_2]$ under knowledge $\eta_A\eta_B$ is 1. The probability is of course 0 if the coordinate relation is not met, so we have in general that

$$\Phi([\eta_1\eta_2]|\eta_A\eta_B) = \delta_{\{\eta_1,\eta_2\},\{\eta_A,\eta_B\}} = \delta_{\eta_1\eta_A} \delta_{\eta_2\eta_B} + \delta_{\eta_1\eta_B} \delta_{\eta_2\eta_A} \quad (7.1.2)$$

where clearly only one of the terms of the sum on the RHS can be nonzero at once. The contemporary bases $\eta_A\eta_B$ and $[\eta_1\eta_2]$ are of the same dimension and we can apply Feynman's law (3.5.1) of Chapter I to give

$$\Phi([\eta_1\eta_2]|Y) = \sum_{\eta_A\eta_B} \Phi([\eta_1\eta_2]|\eta_A\eta_B)\Phi(\eta_A\eta_B|Y). \quad (7.1.3)$$

Substituting (7.1.1) and (7.1.2) in (7.1.3) we find

$$\Phi([\eta_1\eta_2]|Y) = (\Phi_A(\eta_1|Y)\Phi_B(\eta_2|Y) + \Phi_A(\eta_2|Y)\Phi_B(\eta_1|Y))e^{ik} \quad (7.1.4)$$

where only one of the two terms of the sum in the bracket can be nonzero at once.

Hence (7.1.4) is the required relation between wave functions $\Phi([\eta_1\eta_2]|Y)$ and $\Phi_A(\eta_A|Y)\Phi_B(\eta_B|Y)$ holding at any one time t and by the general relation (5.1.4) we have

$$\Phi(\eta_1\eta_2|Y) = \frac{1}{\sqrt{2}} (\Phi_A(\eta_1|Y)\Phi_B(\eta_2|Y) + \Phi_A(\eta_2|Y)\Phi_B(\eta_1|Y))e^{ik} \quad (7.1.5)$$

which is the required relation between the wave functions $\Phi(\eta_1\eta_2|Y)$ and $\Phi_A(\eta_A|Y)\Phi_B(\eta_B|Y)$ also holding at any time t .

7.2 Case of identical fermions

In the case of a pair of well separated *fermions* similar arguments apply. Under pure knowledge Y we may then have wave functions $\Phi_A(\xi_A|Y)$ and $\Phi_B(\xi_B|Y)$, in separate moving regions A and B , where ξ_A and ξ_B are the coordinates of the fermions (specifying the general volume element of space and z component of spin for particles A and B respectively). Our wave function for the pair (in sample space S confined to any one time t) is

$$\Phi(\xi_A\xi_B|Y) = \Phi_A(\xi_A|Y)\Phi_B(\xi_B|Y)e^{ik}. \quad (7.2.1)$$

We again claim that $[\xi_1\xi_2] \overset{0}{\leftrightarrow} \xi_A\xi_B$ when

$(\xi_1 = \xi_A \text{ and } \xi_2 = \xi_B) \text{ or } (\xi_1 = \xi_B \text{ and } \xi_2 = \xi_A)$

giving, for the contemporary bases $[\xi_1 \xi_2]$ and $\xi_A \xi_B$ in S , the transformation function

$$\Phi([\xi_1 \xi_2] | \xi_A \xi_B) = \delta_{\{\xi_1, \xi_2\}, \{\xi_A, \xi_B\}} = \delta_{\xi_1 \xi_A} \delta_{\xi_2 \xi_B} + \delta_{\xi_1 \xi_B} \delta_{\xi_2 \xi_A}. \quad (7.2.2)$$

Feynman's law

$$\Phi([\xi_1 \xi_2] | Y) = \sum_{\xi_A \xi_B} \Phi([\xi_1 \xi_2] | \xi_A \xi_B) \Phi(\xi_B \xi_A | Y)$$

applies and gives, by (7.2.1) and (7.2.2)

$$\Phi([\xi_1 \xi_2] | Y) = (\Phi_A(\xi_1 | Y) \Phi_B(\xi_2 | Y) + \Phi_A(\xi_2 | Y) \Phi_B(\xi_1 | Y)) e^{ik} \quad (7.2.3)$$

This is the required functional relation between $\Phi([\xi_1 \xi_2] | Y)$ and $\Phi_A(\xi_A | Y) \Phi_B(\xi_B | Y)$ holding at any time t . And this relation is an example of a case in which the wave function $\Phi([\xi_1 \dots \xi_N] | Y)$ for fermions is a continuous (and differentiable) function of the continuous components of the coordinates. From the relation (6.1.10) we further have at any time t that

$$\Phi(\xi_1 \xi_2 | Y) = \pm \frac{e^{i\alpha^{(\xi)}}}{\sqrt{2}} (\Phi_A(\xi_1 | Y) \Phi_B(\xi_2 | Y) + \Phi_A(\xi_2 | Y) \Phi_B(\xi_1 | Y)) e^{ik} \quad \begin{cases} \xi_1 < \xi_2 \\ \xi_2 < \xi_1 \end{cases} \quad (7.2.4)$$

where $\alpha^{(\xi)}$ is a constant phase for the dynamic basis ξ and is independent of ξ_1 and ξ_2 , and of t , and where, for example, the plus sign applies when $\xi_1 < \xi_2$ i.e. when ξ_1 comes before ξ_2 in the dynamic order of coordinate values at the time t in question.

We now make the claim that during the motion of the particles, the dynamic order of ξ values of the identical fermions is at any time such that when ξ_1 refers to region A and ξ_2 to region B we have $\xi_1 < \xi_2$. Then of course when ξ_1 refers to region B and ξ_2 to region A we have $\xi_2 < \xi_1$.*

This choice of the dynamic order of ξ values is almost forced by the requirement that $\Phi(\xi_1 \xi_2 | Y)$ in (7.2.4) must be a continuous and differentiable function of the spatial components of the particle coordinates. It certainly ensures that this requirement is fulfilled.†

* We could of course claim instead that when ξ_1 refers to region B and ξ_2 to region A then $\xi_1 < \xi_2$, and therefore when ξ_1 refers to region A and ξ_2 to region B $\xi_2 < \xi_1$.

† Note that if we were to claim generally that the natural 'dynamic order' of ξ values was in fact *constant in time*, the present claim concerning the 'dynamic order', which is more or less forced on us, would lead to

Since the functions $\Phi_A(\xi_1|Y)$, $\Phi_B(\xi_2|Y)$...etc in (7.2.4) are zero outside their regions we can now rewrite (7.2.4) as

$$\Phi(\xi_1\xi_2|Y) = \frac{e^{i\alpha^{(\xi)}}}{\sqrt{2}} (\Phi_A(\xi_1|Y)\Phi_B(\xi_2|Y) - \Phi_A(\xi_2|Y)\Phi_B(\xi_1|Y))e^{ik}. \quad (7.2.5)$$

This is the required relation between the wave functions $\Phi(\xi_1\xi_2|Y)$ and $\Phi_A(\xi_A|Y)\Phi_B(\xi_B|Y)$ in the case of a pair of separated fermions. And it holds at any time t . It is a relation indeterminate only with regard to the unimportant constant phase $\alpha^{(\xi)} + k$ which is conventionally taken to be zero.

7.3 Generalisation

The above theory generalises to the case of any number of bosons (or any number of fermions) in any kind of separate regions of the 4-D (3-D continuous plus 1-D discrete) space spanned by the η (or ξ) coordinates. For example it generalises to the case when we can distinguish a number of fermions because we know their different z components of spin, or to the case when we can distinguish a number of bosons because we know the different z components of spin of some of them and the different regions of space occupied by the others.

7.3.1 Generalised case for bosons

Let the separate (generally moving) regions of the 4-D space be denoted by A_1, \dots, A_N .

Denoting the 'regional' coordinates (in the case of the N bosons) by $\eta_{A_1}, \dots, \eta_{A_N}$ and the non-regional coordinates by η_1, \dots, η_N , and by working in the combined sample space S (of the N particles) confined to any one time t we easily prove that (7.1.2) generalises to

$$\Phi([\eta_1 \dots \eta_N] | \eta_{A_1} \dots \eta_{A_N}) = \sum_P \delta_{\eta_1 \eta_{A_1}} \dots \delta_{\eta_N \eta_{A_N}}$$

where P indicates summation over all the permutations of the η_1, \dots, η_N .

contradiction. For let A' and B' be unmoving regions of fixed space initially coincident with the (moving) regions A and B respectively. The wave packets $\Phi_A(\xi_A|Y)$ and $\Phi_B(\xi_B|Y)$ then initially occupy the (unmoving) regions A' and B' of fixed space and could, after a time, be made (by application of appropriate external fields) to occupy the fixed regions B' and A' respectively. So taking two coordinate values ξ_1 and ξ_2 , with ξ_1 in region A' and ξ_2 in B' , we have initially $\xi_1 < \xi_2$ but finally $\xi_2 < \xi_1$. And this is inconsistent with the dynamic order of ξ values being constant in time.

And using Feynman's law

$$\Phi([\eta_1 \dots \eta_N] | Y) = \sum_{\eta_{A_1} \dots \eta_{A_N}} \Phi([\eta_1 \dots \eta_N] | \eta_{A_1} \dots \eta_{A_N}) \Phi(\eta_{A_1} \dots \eta_{A_N} | Y)$$

with

$$\Phi(\eta_{A_1} \dots \eta_{A_N} | Y) = \Phi_{A_1}(\eta_{A_1} | Y) \dots \Phi_{A_N}(\eta_{A_N} | Y) e^{ik(N-1)}$$

we get

$$\Phi([\eta_1 \dots \eta_N] | Y) = \sum_P \Phi_{A_1}(\eta_{i_1} | Y) \dots \Phi_{A_N}(\eta_{i_N} | Y) e^{ik(N-1)}. \quad (7.3.1.1)$$

Hence by (5.1.4)

$$\Phi(\eta_1 \dots \eta_N | Y) = \frac{1}{\sqrt{N!}} \sum_P \Phi_{A_1}(\eta_{i_1} | Y) \dots \Phi_{A_N}(\eta_{i_N} | Y) e^{ik(N-1)} \quad (7.3.1.2)$$

and this is the required relation between the wave function $\Phi(\eta_1 \dots \eta_N | Y)$ and the wave function $\Phi_{A_1}(\eta_{A_1} | Y) \dots \Phi_{A_N}(\eta_{A_N} | Y)$.

7.3.2 Generalised case for fermions

Now consider a system of N fermions occupying separate regions of 4-D space again denoted by $A_1 \dots A_N$.

Denoting the 'regional' coordinates by $\xi_{A_1}, \dots, \xi_{A_N}$ and the non-regional coordinates by ξ_1, \dots, ξ_N , and again working in the combined sample space S (of the N particles) confined to any one time t , we easily prove that the transformation function in (7.2.2) generalises to

$$\Phi([\xi_1 \dots \xi_N] | \xi_{A_1} \dots \xi_{A_N}) = \delta_{\{\xi_1 \dots \xi_N\}, \{\xi_{A_1} \dots \xi_{A_N}\}} = \sum_P \delta_{\xi_1 \xi_{A_1}} \dots \delta_{\xi_N \xi_{A_N}}$$

where P indicates summation over all the permutations of the ξ_1, \dots, ξ_N .

And using Feynman's law

$$\Phi([\xi_1 \dots \xi_N] | Y) = \sum_{\xi_{A_1} \dots \xi_{A_N}} \Phi([\xi_1 \dots \xi_N] | \xi_{A_1} \dots \xi_{A_N}) \Phi(\xi_{A_1} \dots \xi_{A_N} | Y)$$

with

$$\Phi(\xi_{A_1} \dots \xi_{A_N} | Y) = \Phi_{A_1}(\xi_{A_1} | Y) \dots \Phi_{A_N}(\xi_{A_N} | Y) e^{ik(N-1)}$$

we get

$$\Phi([\xi_{A_1} \dots \xi_{A_N}] | Y) = \sum_P \Phi_{A_1}(\xi_{A_1} | Y) \dots \Phi_{A_N}(\xi_{A_N} | Y) e^{ik(N-1)}. \quad (7.3.2.1)$$

By (6.1.10) we therefore have

$$\Phi(\xi_1 \dots \xi_N | Y) = \pm \frac{e^{i\alpha^{(\xi)}}}{\sqrt{N!}} \sum_P \Phi_{A_1}(\xi_1 | Y) \dots \Phi_{A_N}(\xi_N | Y) e^{ik(N-1)}. \quad (7.3.2.2)$$

where the plus signs applies when the ξ values ξ_1, \dots, ξ_N on the LHS are in the dynamic order or can be put in the dynamic order by an even permutation, and the minus applies when an odd permutation is required.

We now make the claim that the dynamic order of ξ values during the motion of the system of fermions can be taken such that ξ values in separate regions A_1, \dots, A_N of 4-D space are always in ascending order. This means the \pm sign in (7.3.2.2) does not change when the ξ_1, \dots, ξ_N are varied under the constraint that they remain confined to different regions A_1, \dots, A_N . Since only one of the terms of the summand in (7.3.2.2) can be non-zero at once, we can write (7.3.2.2) as

$$\Phi(\xi_1 \dots \xi_N | Y) = \frac{e^{i\alpha^{(\xi)}}}{\sqrt{N!}} \sum_P (\pm) \Phi_{A_1}(\xi_1 | Y) \dots \Phi_{A_N}(\xi_N | Y) e^{ik(N-1)}. \quad (7.3.2.3)$$

where P indicates summation over all permutations of ξ_1, \dots, ξ_N , (\pm) being plus for even permutations and minus for odd permutations.

Thus (7.3.2.3) is the required general relation between the wave function $\Phi(\xi_1 \dots \xi_N | Y)$ and the wave function $\Phi_{A_1}(\xi_{A_1} | Y) \dots \Phi_{A_N}(\xi_{A_N} | Y)$. It is a relation indeterminate only with regard to an unimportant constant phase $\alpha^{(\xi)} + k(N-1)$ which may conventionally be taken to be zero.

8. Wave functions for a number of non-interacting identical particles that start out distinguishable but then become indistinguishable

Suppose we have two identical non-interacting bosons A and B initially well separated in space and, on account of this spatial separation alone, initially distinguishable as in section 7.1. They may possibly be moving under the action of known external potentials but we suppose they never interact with one another even when in time they approach so close to one another as to be no longer distinguishable. Now there are sample spaces S_{σ}^A and S_{σ}^B of propositions about the orbital and spinning motions of each particle over the

time period when they are well separated and distinguishable. For times t in the interval $t_0 < t < t_1$ during which the particles are distinguishable, the sample spaces S_{cr}^A and S_{cr}^B are closed and we suppose we have pure separable knowledge Y of the particle motions represented by time evolving wave functions $\Phi_A(\eta_A|Y)$ and $\Phi_B(\eta_B|Y)$ of the particle coordinates η_A and η_B in sample spaces S_{cr}^A and S_{cr}^B . These wave functions are moving wave packets well separated in space throughout the period $t_0 < t < t_1$. Let us suppose these wave packets would, if they continued to evolve according to the Schrödinger equation, overlap during times $t_1 \leq t < t_2$. Then the particles are no longer distinguishable, and that implies the description of our knowledge by means of wave functions $\Phi_A(\eta_A|Y)$ and $\Phi_B(\eta_B|Y)$ in sample spaces S_{cr}^A and S_{cr}^B , or by means of the wave function $\Phi(\eta_A\eta_B|Y) = \Phi_A(\eta_A|Y)\Phi_B(\eta_B|Y)e^{ik}$ in the sample space $S_{cr}^A S_{cr}^B$, is no longer applicable.

Nonetheless we still have pure knowledge Y of the motion of the pair of particles in a sample space S (for the pair of particles covering times from t_0 onwards) which is closed in relation to other sample spaces. This pure knowledge can be represented by a wave function $\Phi(\eta_1\eta_2|Y)$ in S , where η_1 and η_2 are respectively the coordinates of the earliest particle in the natural order of particles and the remaining particle. The derivation of the expression (7.1.5) for this wave function in terms of the functions $\Phi_A(\eta_A|Y)$ and $\Phi_B(\eta_B|Y)$ is still valid during times $t_0 < t < t_1$ and, if we formally allow the functions $\Phi_A(\eta_A|Y)$, $\Phi_B(\eta_B|Y)$ to continue to evolve according to the Schrödinger equations as if each particle was on its own, $\Phi(\eta_1\eta_2|Y)$ (as given by (7.1.5)) will also continue to satisfy the Schrödinger equation (in coordinates $\eta_1\eta_2$) for the particle pair. Therefore (7.1.5) is also valid during times $t_1 \leq t < t_2$ when the individual wave packets overlap and it serves perfectly well to express our pure state of knowledge in sample space S covering the whole period $t_0 < t < t_2$.

From (7.1.5) we may work out the modulus squared of $\Phi(\eta_1\eta_2|Y)$ getting

$$\begin{aligned} |\Phi(\eta_1\eta_2|Y)|^2 = \frac{1}{2} & \left(|\Phi_A(\eta_1|Y)\Phi_B(\eta_2|Y)|^2 + |\Phi_A(\eta_2|Y)\Phi_B(\eta_1|Y)|^2 \right. \\ & + \Phi_A^*(\eta_1|Y)\Phi_B^*(\eta_2|Y)\Phi_A(\eta_2|Y)\Phi_B(\eta_1|Y) \\ & \left. + \Phi_A^*(\eta_2|Y)\Phi_B^*(\eta_1|Y)\Phi_A(\eta_1|Y)\Phi_B(\eta_2|Y) \right) \end{aligned} \quad (8.1)$$

valid at any time during the process. In (8.1) the ‘interference terms’ are for certain zero only during the time $t_0 < t < t_1$ when the wave packets do not overlap.

Now (8.1) gives, at any time t in the interval $t_0 < t < t_2$, the expected frequency in repeated trials for the earliest particle (in the natural order of particles) to have coordinates η_1 and the other particle to have coordinates η_2 (see section 9 of Chapter II).

This is not a frequency that can be checked experimentally even if we could by chance get to know the coordinates of the particles at time t because the natural order of the particles could not be ascertained. It is nonetheless an expected frequency.

If we were to suppose (contrary to the assertion near the end of section 3.6 of Chapter III) that we *could* claim to know the natural order of identical particles on any occasion, then, for any specified values of η_1 and η_2 , we could, in a large number of trials, come up with an ‘observed’ frequency at which the earliest particle in the ‘natural’ order had coordinates η_1 and the other particle coordinates η_2 . But being dependent on the choice of order made on each occasion the coordinates η_1 and η_2 were found to be occupied, this frequency would be ambiguous and would generally differ from the expected frequency as given by (8.1). There is therefore good reason for maintaining the rule that we *cannot* claim to know the natural order of identical particles when they are not clearly distinguishable throughout the process considered.

From the general relation (5.1.3) we have from (8.1), that

$$\begin{aligned} |\Phi([\eta_1\eta_2]|Y)|^2 &= (2 - \delta_{\eta_1, \eta_2}) |\Phi(\eta_1\eta_2|Y)|^2 \\ &= (1 - \frac{1}{2} \delta_{\eta_1, \eta_2}) \left(|\Phi_A(\eta_1|Y)\Phi_B(\eta_2|Y)|^2 + |\Phi_A(\eta_2|Y)\Phi_B(\eta_1|Y)|^2 \right. \\ &\quad + \Phi_A^*(\eta_1|Y)\Phi_B^*(\eta_2|Y)\Phi_A(\eta_2|Y)\Phi_B(\eta_1|Y) \\ &\quad \left. + \Phi_A^*(\eta_2|Y)\Phi_B^*(\eta_1|Y)\Phi_A(\eta_1|Y)\Phi_B(\eta_2|Y) \right) \quad \dots(8.2) \end{aligned}$$

and this equals the expected frequency, at time t , for one or other particle to have coordinates η_1 and the other to have coordinates η_2 . This frequency *can* be checked experimentally whenever the coordinates can by chance be measured, i.e. whenever $[\eta_1\eta_2]$ is a *primary* basis.

When we can check an expected frequency in quantum mechanics we expect to get agreement with theory. And we generally do. But this only means expected frequencies (properly calculated from probabilities) are generally found to be close enough to the frequencies at which the events in question are observed in a large number of trials. It does not imply the latter frequencies are *predictable* i.e. determined from the physical conditions we know to be present. Should we assume they *were*, we might be led falsely to claim that the expected frequency for one or other particle to have coordinates η_1 and the other coordinates η_2 was simply

$$|\Phi([\eta_1\eta_2]|Y)|^2 = (1 - \frac{1}{2} \delta_{\eta_1, \eta_2}) \left(|\Phi_A(\eta_1|Y)\Phi_B(\eta_2|Y)|^2 + |\Phi_A(\eta_2|Y)\Phi_B(\eta_1|Y)|^2 \right)$$

on the grounds that, because the particles do not interact, this frequency is to be calculated directly from the frequencies $|\Phi_A(\eta_A|Y)|^2$ and $|\Phi_B(\eta_B|Y)|^2$ predicted for each particle moving separately. But this would be false reasoning, i.e. reasoning outside the logical and physical rules of quantum mechanics. And in practice we generally get close enough agreement between expected and observed frequencies only when the ‘interference terms’ in (8.2) are included.

The above method for deriving the expected frequencies (8.2) of coordinate values for a pair of non-interacting identical bosons can clearly be generalised to the case of a system of any number of non-interacting identical bosons or fermions (possibly moving under the action of an external potential field) that start out distinguishable and then become indistinguishable. In the case of bosons we make use of the result (7.3.1.2) (valid when the bosons are distinguishable) and use it to calculate the improper wave function $\Phi(\eta_1 \dots \eta_N | Y)$ for all time. From this we can get the proper wave function $\Phi([\eta_1 \dots \eta_N] | Y)$ for all time using the general relation (5.1.3). In the case of fermions we make use of the result (7.3.2.3) and use it to calculate the improper wave function $\Phi(\xi_1 \dots \xi_N | Y)$ for all time. From this we can get the proper wave function $\Phi([\xi_1 \dots \xi_N] | Y)$ for all time using the general relation (6.1.10). We then take the squared moduli of the proper wave functions to get the expected frequencies.

8.1 Possibility of a return to distinguishable particles

Identical particles that start out distinguishable, from time t_0 to time t_1 and become indistinguishable from time t_1 to t_2 , may become distinguishable again from time t_2 onwards.

For example the two identical bosons A and B above that started out distinguishable with our pure states of knowledge of each represented by the spatially separated but converging wave packets $\Phi_A(\eta_A | Y)$ and $\Phi_B(\eta_B | Y)$ may become distinguishable again from time t_2 onward when those packets, each formally evolving according to its own Schrödinger equation, have become (for ever) spatially separated again.

In the sample space S covering motion of the two particles from time t_0 to infinity, the valid representation of our pure knowledge is afforded by the improper wave function $\Phi(\eta_1 \eta_2 | Y)$ (as given by (7.1.5)). After time t_2 when the wave packets A and B have separated again, and with respect to the sample space S covering times from t_2 onward, we are at liberty to claim to know which particle (in the natural order of particles) occupies packet A and which occupies packet B . Let Z_1 and Z_2 denote the propositions claiming respectively that the particle in packet A is occurring *first* and *second* in the natural order of particles.*

If at time t_2 we choose to claim the truth of Z_1 , then Z_1 becomes part of our knowledge of dynamical properties and we are performing (action-less) harmless conditioning over the basis $\eta_1 \eta_2$ in S . Our wave function accordingly changes to $\Phi(\eta_1 \eta_2 | Z_1 Y)$ given by

* Of course, if Z_1 (or Z_2) is true at time t_2 it will be true any time thereafter. For the particles clearly cannot change places in any infinitesimal time (say from t to $t + dt$) without moving infinitely fast.

$$\Phi(\eta_1\eta_2|Z_1Y) = \begin{cases} \frac{\Phi(\eta_1\eta_2|Y)}{\Phi(Z_1|Y)} e^{-ik} & \eta_1 \in A \\ 0 & \eta_1 \notin A \end{cases} \quad (8.1.1)$$

where k is the phase characteristic of knowledge Y and A denotes the region of 8-D (2×3 -D continuous plus 2×1 -D discrete) $\eta_1\eta_2$ space occupied by wave packet A . The probabilities $\Phi(Z_1|Y)$ and $\Phi(Z_2|Y)$ are, by the principle of indifference,

$$\Phi(Z_1|Y) = \frac{1}{\sqrt{2}} e^{i(\alpha_1-k)}, \quad \Phi(Z_2|Y) = \frac{1}{\sqrt{2}} e^{i(\alpha_2-k)} \quad (8.1.2)$$

where the phases α_1 and α_2 characteristic of Z_1 and Z_2 under knowledge Y are indeterminate. Substituting (from (7.1.5)) for the wave function $\Phi(\eta_1\eta_2|Y)$ and (from (8.1.2)) for $\Phi(Z_1|Y)$, (8.1.1) becomes

$$\Phi(\eta_1\eta_2|Z_1Y) = \sqrt{2} e^{-i(\alpha_1-k)} \cdot \frac{1}{\sqrt{2}} (\Phi_A(\eta_1|Y)\Phi_B(\eta_2|Y) + \Phi_A(\eta_2|Y)\Phi_B(\eta_1|Y)) e^{ik} e^{-ik}$$

when $\eta_1 \in A$ and zero otherwise. The second term in the brackets is clearly zero when $\eta_1 \in A$, and renaming the particle coordinates η_A and η_B instead of η_1 and η_2 we have

$$\Phi(\eta_A\eta_B|Z_1Y) = \Phi_A(\eta_A|Y)\Phi_B(\eta_B|Y) e^{-i\alpha_1} e^{ik} \quad (8.1.3)$$

for our probability distribution over the basis $\eta_A\eta_B$ in S for $t > t_2$.

The distribution (8.1.3) clearly qualifies as a wave function showing Z_1Y represents a pure state of knowledge, and because it factors, we hold a pure state of knowledge with regard to particle A in $S_{\sigma r}^A$ with wave function $\Phi_A(\eta_A|Y)$ (to within a constant phase factor) and a pure state of knowledge with regard to particle B in $S_{\sigma r}^B$ with wave function $\Phi_B(\eta_B|Y)$ (to within a constant phase factor).

Note however that it is not possible to prove that if η_1 was in fact in the region of configuration space occupied by wave packet A *initially* (i.e. for $t_0 < t < t_1$) it would necessarily have *finally* (i.e. for $t > t_2$) to be in the region of configuration space occupied by the same (time evolved) wave packet A .

CHAPTER XI

TIME REVERSAL, PARITY AND STATIONARY STATES

1. The change in wave function under time reversal *

Corresponding to any pure state of knowledge YG relating to a quantum mechanical process there is a pure state of knowledge $\tilde{Y}\tilde{G}$ relating to a time reversed version of the process. On passing from a pure state of knowledge YG to its time reversed form $\tilde{Y}\tilde{G}$ the wave function expressing our knowledge changes in a certain way, sometimes simply to its complex conjugate with the sign of the time changed. We show how the change in wave function can be calculated in specific cases. When applied twice, this change in wave function must return the wave function to its original form because (as noted in section 3.11 of Chapter III) any process time reversed twice is the same as the original process.

1.1 Case of orbital motion of a particle moving under the action of general potentials

Relative to a fixed coordinate system, the law of time reversal (section 3.11 of Chapter III) implies that to every possible motion $\mathbf{r} = \mathbf{f}(t)$ of the particle under potentials $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ there is possible motion $\mathbf{r} = \mathbf{f}(-t)$ under potentials $V(\mathbf{r}, -t)$ and $-\mathbf{A}(\mathbf{r}, -t)$. Let our general knowledge G and (on another occasion) \tilde{G} differ only with regard to our knowledge of the potentials. So under G suppose we know that the potentials are $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$, and under \tilde{G} suppose we know that the potentials are $V(\mathbf{r}, -t)$ and $-\mathbf{A}(\mathbf{r}, -t)$.

Let our pure knowledge YG be expressed by a wave function $\psi(\mathbf{r}, 0)$ at time $t = 0$ in a (closed) sample space S of all propositions about the particle motion in a time period $-t_0 < t < t_0$. During the time period covered by the sample space $\psi(\mathbf{r}, t)$ obeys the Schrödinger equation (4.2.4) of Chapter IV. With the calculated values of α, β, γ and ε this equation is

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi + \frac{i\hbar}{m} \mathbf{A} \cdot \nabla \psi + \frac{1}{2m} A^2 \psi, \quad (1.1.1)$$

* When we speak of 'time reversal' we do not of course mean that time itself is reversed. We refer instead to physical processes that take place in reverse.

Now corresponding to YG , time reversed pure knowledge $\tilde{Y}\tilde{G}$ is pure knowledge that is consistent with the particle motion being reversed.* And by of the law of time reversal (in section 3.11 of Chapter III), for every possible motion $\mathbf{r} = \mathbf{f}(t)$ consistent with knowledge YG , there corresponds, under $\tilde{Y}\tilde{G}$ a possible motion $\mathbf{r} = \mathbf{f}(-t)$ consistent with knowledge $\tilde{Y}\tilde{G}$ and vice versa. So for any possible value $\mathbf{r} = \mathbf{r}_1$ at t_1 (under knowledge YG) resulting from one or other orbit $\mathbf{r} = \mathbf{f}(t)$ (with $\mathbf{f}(t_1) = \mathbf{r}_1$) there corresponds the same value $\mathbf{r} = \mathbf{r}_1$ at $-t_1$ (under $\tilde{Y}\tilde{G}$) resulting from the (time-reversed) orbit $\mathbf{r} = \mathbf{f}(-t)$ (since $\mathbf{f}(-(-t_1)) = \mathbf{r}_1$). And accordingly we claim the problem of finding $\tilde{\psi}(\mathbf{r}, t)$ at any time t ($-t_0 < t < t_0$) under knowledge $\tilde{Y}\tilde{G}$ is *similar* to that of finding $\psi(\mathbf{r}, t)$ at time $-t$ under knowledge YG .

Therefore, by the similarity principle ((5.1.2) of Chapter I and its alternative form (8.1.2) of Chapter I) we should set either

$$\tilde{\psi}(\mathbf{r}, t) = \psi^*(\mathbf{r}, -t) \quad (1.1.2)$$

or

$$\tilde{\psi}(\mathbf{r}, t) = \psi(\mathbf{r}, -t)e^{i\alpha} \quad (1.1.3)$$

where the real number α is independent of \mathbf{r} and t , and of the particular functions $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$.

But the wave function $\tilde{\psi}(\mathbf{r}, t)$ must also satisfy the Schrödinger equation (1.1.1) with $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ changed to $V(\mathbf{r}, -t)$ and $-\mathbf{A}(\mathbf{r}, -t)$. This is true of (1.1.2) but not of (1.1.3).

To see this we start by changing the sign of the time in (1.1.1). This gives

$$\begin{aligned} \frac{\hbar}{i} \frac{\partial \psi(\mathbf{r}, -t)}{\partial t} = & -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, -t) + V(\mathbf{r}, -t) \psi(\mathbf{r}, -t) + \frac{i\hbar}{m} \mathbf{A}(\mathbf{r}, -t) \cdot \nabla \psi(\mathbf{r}, -t) \\ & + \frac{1}{2m} A(\mathbf{r}, -t)^2 \psi(\mathbf{r}, -t) \end{aligned} \quad \dots(1.1.4)$$

Taking the conjugate of this equation confirms that $\psi^*(\mathbf{r}, -t)$ unconditionally satisfies the Schrödinger equation with $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ changed to $V(\mathbf{r}, -t)$ and $-\mathbf{A}(\mathbf{r}, -t)$.

But in order for $\psi(\mathbf{r}, -t)e^{i\alpha}$ to satisfy the Schrödinger equation with $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ changed to $V(\mathbf{r}, -t)$ and $-\mathbf{A}(\mathbf{r}, -t)$, i.e. in order for

* For example, if Y is the pure knowledge that the particle is at $\mathbf{r} = \mathbf{r}_0$ at time $-t_0$ then \tilde{Y} can be expressed as the pure knowledge that the particle is at $\mathbf{r} = \mathbf{r}_0$ at time t_0 .

$$\begin{aligned}
 -\frac{\hbar}{i} \frac{\partial \psi(\mathbf{r}, -t)}{\partial t} = & -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, -t) + V(\mathbf{r}, -t) \psi(\mathbf{r}, -t) - \frac{i\hbar}{m} \mathbf{A}(\mathbf{r}, -t) \cdot \nabla \psi(\mathbf{r}, -t) \\
 & + \frac{1}{2m} A(\mathbf{r}, -t)^2 \psi(\mathbf{r}, -t)
 \end{aligned}
 \tag{1.1.5}$$

to hold we require, by addition of (1.1.4) and (1.1.5) followed by division by 2, that

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, -t) + V(\mathbf{r}, -t) \psi(\mathbf{r}, -t) + \frac{1}{2m} A(\mathbf{r}, -t)^2 \psi(\mathbf{r}, -t) = 0
 \tag{1.1.6}$$

and, by subtracting this from (1.1.4), that

$$\frac{\hbar}{i} \frac{\partial \psi(\mathbf{r}, -t)}{\partial t} = \frac{i\hbar}{m} \mathbf{A}(\mathbf{r}, -t) \cdot \nabla \psi(\mathbf{r}, -t).
 \tag{1.1.7}$$

And (1.1.6) and (1.1.7) must hold for all $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$. But then putting $\mathbf{A}(\mathbf{r}, t) = 0$ would force $\psi(\mathbf{r}, -t)$ and $V(\mathbf{r}, t)$ to be independent of t neither of which is generally true. Therefore option (1.1.3) is ruled out and we conclude that relation (1.1.2) is the correct relation between $\tilde{\psi}(\mathbf{r}, t)$ and $\psi(\mathbf{r}, t)$.

If, using (5.1) of Chapter VI, we work out the wave functions in momentum space corresponding to $\tilde{\psi}(\mathbf{r}, t)$ and $\psi(\mathbf{r}, t)$ we find these are related thus:

$$\tilde{a}(\mathbf{p}, t) = a^*(-\mathbf{p}, -t)
 \tag{1.1.8}$$

which is consistent with the claim that the problem of finding $\tilde{a}(\mathbf{p}, t)$ under knowledge $\tilde{Y}\tilde{G}$ is *similar* to that of finding $a(-\mathbf{p}, -t)$ under knowledge YG .

1.2 Case of spinning motion of a spin one-half particle in a uniform magnetic field

In this case, a wave function under any pure knowledge Y must satisfy the Schrödinger equation (8.2.3) of Chapter VII. With respect to any fixed Cartesian coordinate system O and with $\psi(\sigma, t) = \Phi(\sigma t | Y)$ this equation can be written as

$$i\hbar \frac{\partial \psi(\sigma, t)}{\partial t} = \sum_{\sigma'} H_{\sigma\sigma'}(t) \psi(\sigma', t)
 \tag{1.2.1}$$

where

$$H_{\sigma\sigma'}(t) = -\mu (\sigma_{\sigma\sigma'}^x H_x(t) + \sigma_{\sigma\sigma'}^y H_y(t) + \sigma_{\sigma\sigma'}^z H_z(t)) \quad (1.2.2)$$

μ being the magnetic moment of the particle, $H_i(t)$ ($i=x, y, z$) the Cartesian components (in O) of the uniform but generally time dependent magnetic field, and $\sigma_{\sigma\sigma'}^i$ ($i=x, y, z$) the Pauli matrices (as in (8.2.5) of Chapter VII).

Let us work in the sample space S of all propositions regarding the z components of spin in all fixed coordinate systems in the time period $-t_0 < t < t_0$. Now pure knowledge Y is represented by the wave function $\psi(\sigma, 0)$ and can be, and we assume *is* expressed as knowledge of the value of the z component of spin at time $t=0$ in some fixed Cartesian coordinate system C (not necessarily the same as O).^{*} And our general knowledge G includes knowledge of the field components $H_i(t)$ ($i=x, y, z$) in O during the time period $-t_0 < t < t_0$.

Let \tilde{C} be the coordinate system formed by rotating C through an angle $+\pi$ about the y axis of C . Similarly let \tilde{O} be the coordinate system formed by rotating O through the *same* angle about the y axis of O .

Suppose knowledge \tilde{Y} differs from Y just because the same known value of z component of spin refers to \tilde{C} rather than C . And suppose \tilde{G} differs from G just because the magnetic field $\mathbf{H}(t)$ has become $-\mathbf{H}(-t)$. Then on account of the law of time reversal for spin (in section 3.11 of Chapter III) we claim that the problem of finding the wave function $\tilde{\psi}(\sigma, t)$ at time t in \tilde{O} under knowledge $\tilde{Y}\tilde{G}$ is *similar* to that of finding the wave function $\psi(\sigma, t)$ at time $-t$ in O under knowledge YG . Therefore, by the similarity principle ((5.1.2) of Chapter I) including its extension ((8.1.2) of Chapter I) we should set either

$$\tilde{\psi}(\sigma, t) = \psi^*(\sigma, -t) \quad (1.2.3)$$

or

$$\tilde{\psi}(\sigma, t) = \psi(\sigma, -t)e^{i\alpha} \quad (1.2.4)$$

where the real number α is independent of σ and t , and independent of the function $\mathbf{H}(t)$.

But the wave function $\tilde{\psi}(\sigma, t)$ must also satisfy the Schrödinger equation (1.2.1) in \tilde{O} with $\mathbf{H}(t)$ changed to $-\mathbf{H}(-t)$. This is true of (1.2.3) but not of (1.2.4) as is shown as follows.

The function $\psi(\sigma, t)$ satisfies (1.2.1). On changing the sign of the time this gives

^{*} For proof of the generality of wave function $\psi(\sigma, 0)$ defined in this way see section 6 of Chapter VII.

$$-i\hbar \frac{\partial \psi(\sigma, -t)}{\partial t} = \sum_{\sigma'} H_{\sigma\sigma'}(-t) \psi(\sigma', -t) \quad (1.2.5)$$

where

$$H_{\sigma\sigma'}(-t) = -\mu(\sigma_{\sigma\sigma'}^x H_x(-t) + \sigma_{\sigma\sigma'}^y H_y(-t) + \sigma_{\sigma\sigma'}^z H_z(-t)) \quad (1.2.6)$$

Taking the conjugate of (1.2.5) we find

$$i\hbar \frac{\partial \psi^*(\sigma, -t)}{\partial t} = \sum_{\sigma'} H_{\sigma\sigma'}^*(-t) \psi^*(\sigma', -t) \quad (1.2.7)$$

where, on account of $\sigma_{\sigma\sigma'}^y$ having purely imaginary elements

$$H_{\sigma\sigma'}^*(-t) = -\mu(\sigma_{\sigma\sigma'}^x H_x(-t) - \sigma_{\sigma\sigma'}^y H_y(-t) + \sigma_{\sigma\sigma'}^z H_z(-t)). \quad (1.2.8)$$

The Schrödinger equation for $\tilde{\psi}(\sigma, t)$ in $\tilde{\mathcal{O}}$ with $\mathbf{H}(t)$ changed to $-\mathbf{H}(-t)$ (which means, in $\tilde{\mathcal{O}}$, that $H_x(t)$ and $H_z(t)$ become $H_x(-t)$ and $H_z(-t)$ while $H_y(t)$ becomes $-H_y(-t)$) is

$$i\hbar \frac{\partial \tilde{\psi}(\sigma, t)}{\partial t} = \sum_{\sigma'} \tilde{H}_{\sigma\sigma'}(t) \tilde{\psi}(\sigma', t) \quad (1.2.9)$$

where

$$\tilde{H}_{\sigma\sigma'}(t) = -\mu(\sigma_{\sigma\sigma'}^x H_x(-t) - \sigma_{\sigma\sigma'}^y H_y(-t) + \sigma_{\sigma\sigma'}^z H_z(-t)). \quad (1.2.10)$$

So comparison of equations (1.2.7) and (1.2.8) with equations (1.2.9) and (1.2.10) shows that with the choice (1.2.3), $\tilde{\psi}(\sigma, t)$ unconditionally satisfies the Schrödinger equation in $\tilde{\mathcal{O}}$ when $\mathbf{H}(t)$ is changed to $-\mathbf{H}(-t)$.

But for $\psi(\sigma, -t)e^{i\alpha}$ to satisfy (1.2.9) we require

$$i\hbar \frac{\partial \psi(\sigma, -t)}{\partial t} = \sum_{\sigma'} \tilde{H}_{\sigma\sigma'}(t) \psi(\sigma', -t) \quad (1.2.11)$$

and adding this to (1.2.5) gives

$$\sum_{\sigma'} (H_{\sigma\sigma'}(-t) + \tilde{H}_{\sigma\sigma'}(t)) \psi(\sigma', -t) = 0$$

or

$$-\mu \sum_{\sigma'} (\sigma_{\sigma\sigma'}^x H_x(-t) + \sigma_{\sigma\sigma'}^z H_z(-t)) \psi(\sigma', -t) = 0 \quad (1.2.12)$$

and subtracting this from (1.2.11) gives

$$i\hbar \frac{\partial \psi(\sigma, -t)}{\partial t} = \mu \sum_{\sigma'} \sigma_{\sigma\sigma'}^y H_y(-t) \psi(\sigma', -t). \quad (1.2.13)$$

and (1.2.12) and (1.2.13) must hold for all $\mathbf{H}(t)$. But putting $H_x(t)$ and $H_y(t)$ equal to zero then forces $\psi(\sigma, -t)$ to be constant (in (1.2.13) and forces $H_z(t)$ to be zero (in (1.2.12)) when $\psi(\frac{1}{2}, -t) \neq \psi(-\frac{1}{2}, -t)$, and neither of these is generally true. Therefore option (1.2.4) must be rejected and (1.2.3) gives the required change in wave function under time reversal in the case of spinning motion of a spin one-half particle in a uniform magnetic field.

True, the new wave function refers to a new coordinate system (to $\tilde{\mathbf{O}}$ rather than \mathbf{O}) but we can find the new wave function (call it $\psi'(\sigma, t)$) in the original coordinate system \mathbf{O} simply by applying the transformation rule (3.6) of Chapter VII. In its inverse form this gives us

$$\begin{pmatrix} \psi'(\frac{1}{2}) \\ \psi'(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix} \begin{pmatrix} \tilde{\psi}(\frac{1}{2}) \\ \tilde{\psi}(-\frac{1}{2}) \end{pmatrix}$$

where, when $\tilde{\mathbf{O}}$ is formed by rotating \mathbf{O} through the angle $+\pi$ about the y axis, the Euler angles determining the values of the matrix elements are $(\alpha, \beta, \gamma) = (\pi, 0, -\pi)$. Accordingly

$$\begin{pmatrix} \psi'(\frac{1}{2}) \\ \psi'(-\frac{1}{2}) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \tilde{\psi}(\frac{1}{2}) \\ \tilde{\psi}(-\frac{1}{2}) \end{pmatrix}$$

so the time reversed wave function (given by (1.2.3) in $\tilde{\mathbf{O}}$) is

$$\psi'(\sigma, t) = \psi^*(-\sigma, -t) (-1)^{\frac{1}{2}-\sigma} \quad (1.2.14)$$

in \mathbf{O} .*

* cf. equation (60.2) of [12] in which (typographically) conjugation of $\psi_{s,-\sigma}$ on the RHS is missing

2. The change in wave function under inversion

Corresponding to any pure state of knowledge YG relating to a quantum mechanical process there is clearly a pure state of knowledge $\tilde{Y}\tilde{G}$ relating to an inverted version of the process. On passing from a pure state of knowledge YG to its inverted form $\tilde{Y}\tilde{G}$ any wave function expressing our knowledge of the process changes in a certain way, often simply by a change in sign of its independent dynamical variables. As in the case of time reversal we show how the change in wave function can be calculated in specific cases.

2.1 Case of orbital motion of a particle moving under the action of general potentials

Relative to a fixed coordinate system, the law of inversion (section 3.11 of Chapter III) implies that to every possible motion $\mathbf{r} = \mathbf{f}(t)$ of the particle under potentials $V(\mathbf{r}, t)$ and $A(\mathbf{r}, t)$ there is possible motion $\mathbf{r} = -\mathbf{f}(t)$ under potentials $V(-\mathbf{r}, t)$ and $-A(-\mathbf{r}, t)$. Let G include the general knowledge that the potentials are $V(\mathbf{r}, t)$ and $A(\mathbf{r}, t)$, and let \tilde{G} include instead the general knowledge that the potentials are $V(-\mathbf{r}, t)$ and $-A(-\mathbf{r}, t)$.

Let our pure knowledge YG be expressed by a wave function $\psi(\mathbf{r}, 0)$ at time $t=0$ in a (closed) sample space S of all propositions about the particle motion in a time period $0 < t < t_1$. During this time period $\psi(\mathbf{r}, t)$ obeys the Schrödinger equation (1.1.1).

Now corresponding to the pure knowledge Y , the inverted form \tilde{Y} must be pure knowledge consistent with the particle motion being inverted.* And by the law of inversion (in section 3.11 of Chapter III) for every possible motion $\mathbf{r} = \mathbf{f}(t)$ consistent with knowledge YG , there corresponds the motion $\mathbf{r} = -\mathbf{f}(t)$ consistent with knowledge $\tilde{Y}\tilde{G}$ and vice versa. We thus claim the problem of finding the wave function $\tilde{\psi}(\mathbf{r}, t)$ at \mathbf{r} under knowledge $\tilde{Y}\tilde{G}$ is *similar* to that of finding the wave function $\psi(\mathbf{r}, t)$ at $-\mathbf{r}$ under knowledge YG . Therefore, by the similarity principle ((5.1.2) of Chapter I and its alternative form (8.1.2) of Chapter I) we should set either

$$\tilde{\psi}(\mathbf{r}, t) = \psi^*(-\mathbf{r}, t) \quad (2.1.1)$$

or

$$\tilde{\psi}(\mathbf{r}, t) = \psi(-\mathbf{r}, t)e^{i\alpha} \quad (2.1.2)$$

where the real number α is independent of \mathbf{r} and t and of the functions $V(\mathbf{r}, t)$ and $A(\mathbf{r}, t)$.

* For example, Y is the pure knowledge that the particle is at $\mathbf{r} = \mathbf{r}_0$ at time $t = 0$ then knowledge \tilde{Y} can be expressed as knowledge that the particle is at $\mathbf{r} = -\mathbf{r}_0$ at time $t = 0$.

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But the wave function $\tilde{\psi}(\mathbf{r}, t)$ must also satisfy the Schrödinger equation (1.1.1) with $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ changed to $V(-\mathbf{r}, t)$ and $-\mathbf{A}(-\mathbf{r}, t)$. This is true of (2.1.2) but not of (2.1.1).

To see this we start by changing the sign of \mathbf{r} in (1.1.1). This gives

$$\begin{aligned} -\frac{\hbar}{i} \frac{\partial \psi(-\mathbf{r}, t)}{\partial t} = & -\frac{\hbar^2}{2m} \nabla^2 \psi(-\mathbf{r}, t) + V(-\mathbf{r}, t) \psi(-\mathbf{r}, t) - \frac{i\hbar}{m} \mathbf{A}(-\mathbf{r}, t) \cdot \nabla \psi(-\mathbf{r}, t) \\ & + \frac{1}{2m} A(-\mathbf{r}, t)^2 \psi(-\mathbf{r}, t) \end{aligned} \quad \dots(2.1.3)$$

which confirms that $\psi(-\mathbf{r}, t)e^{i\alpha}$ satisfies the Schrödinger equation with $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ changed to $V(-\mathbf{r}, t)$ and $-\mathbf{A}(-\mathbf{r}, t)$.

But in order for $\psi^*(-\mathbf{r}, t)$ to satisfy the Schrödinger equation with $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ changed to $V(-\mathbf{r}, t)$ and $-\mathbf{A}(-\mathbf{r}, t)$, i.e. in order for

$$\begin{aligned} -\frac{\hbar}{i} \frac{\partial \psi^*(-\mathbf{r}, t)}{\partial t} = & -\frac{\hbar^2}{2m} \nabla^2 \psi^*(-\mathbf{r}, t) + V(-\mathbf{r}, t) \psi^*(-\mathbf{r}, t) - \frac{i\hbar}{m} \mathbf{A}(-\mathbf{r}, t) \cdot \nabla \psi^*(-\mathbf{r}, t) \\ & + \frac{1}{2m} A(-\mathbf{r}, t)^2 \psi^*(-\mathbf{r}, t) \end{aligned} \quad \dots(2.1.4)$$

to hold we require, by addition of (2.1.3) and the conjugate of (2.1.4) and division by 2, that

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(-\mathbf{r}, t) + V(-\mathbf{r}, t) \psi(-\mathbf{r}, t) + \frac{1}{2m} A(-\mathbf{r}, t)^2 \psi(-\mathbf{r}, t) = 0 \quad (2.1.5)$$

and, by subtracting this from (2.1.3), that

$$-\frac{\hbar}{i} \frac{\partial \psi(-\mathbf{r}, t)}{\partial t} = -\frac{i\hbar}{m} \mathbf{A}(-\mathbf{r}, t) \cdot \nabla \psi(-\mathbf{r}, t). \quad (2.1.6)$$

And (2.1.5) and (2.1.6) must hold for all $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$. But then putting $\mathbf{A}(\mathbf{r}, t) = 0$ would force $\psi(-\mathbf{r}, t)$ and $V(\mathbf{r}, t)$ to be independent of t neither of which is generally true. Therefore option (2.1.1) is ruled out leaving (2.1.2) as the only possibility.

If, using (5.1) of Chapter VI, we work out the wave functions in momentum space corresponding to $\tilde{\psi}(\mathbf{r}, t)$ and $\psi(\mathbf{r}, t)$ we find these are related thus:

$$\tilde{a}(\mathbf{p}, t) = a(-\mathbf{p}, t)e^{i\alpha} \quad (2.1.7)$$

which is consistent with the claim that the problem of finding $\tilde{a}(\mathbf{p}, t)$ under knowledge $\tilde{Y}\tilde{G}$ is *similar* to that of finding $a(-\mathbf{p}, t)$ under knowledge YG .

2.2 Case of spinning motion of a spin one-half particle in a uniform magnetic field

In this case, as we have said in section 1.2, a wave function under any pure knowledge Y must satisfy the Schrödinger equation (1.2.1) with the Hamiltonian in (1.2.2).

As before, pure knowledge Y can be expressed as knowledge of the value of the z component of spin at time $t=0$ in some fixed Cartesian coordinate system C (not necessarily the same as O). And our general knowledge G includes knowledge of the field components $H_i(t)$ ($i = x, y, z$) in O .

It is clear that under inversion, because the spinning motion does not change, knowledge \tilde{Y} is the same as knowledge Y and, because the magnetic field does not change, on account of it being uniform, knowledge \tilde{G} is the same as knowledge G .

Therefore, by the second uniqueness principle in section 5 of Chapter I, we have simply

$$\tilde{\psi}(\sigma, t) = \psi(\sigma, t) \quad (2.2.1)$$

i.e. our wave function remains the same on inversion.

2.3 Parity

In the case of *any* one quantum mechanical process it can likewise be demonstrated that under inversion the wave function (in the particle position/spin representation) undergoes a change in sign of all the particle position coordinates and generally gets multiplied (as in (2.1.2)) by a constant phase factor $e^{i\alpha}$ independent of the position/spin coordinates, and of the potential functions and magnetic field and our state of knowledge of dynamical properties (before inversion). Because of the nature of inversion, if we invert a process a second time we return to the original process. So it must be that our wave function returns exactly to its original form. Hence $(e^{i\alpha})^2$ must equal 1 or

$$e^{i\alpha} = \pm 1 \quad (2.3.1)$$

If we can show $e^{i\alpha} = 1$ we say our knowledge regarding the process has ‘parity 1’ (or ‘even parity’), and if we can show $e^{i\alpha} = -1$ we say our knowledge has ‘parity -1 ’ (or ‘odd parity’).

If the system potential and external potentials for each particle and the magnetic field *remain the same* under inversion*, so our general knowledge stays the same, and if our (pure) knowledge Y is knowledge of a dynamical property that also does not change under inversion, then our wave function must stay the same under inversion.† And accordingly, on changing the sign of the position coordinates our wave function must stay the same (in the case of even parity) or change sign (in the case of odd parity).

For example, in the case of a single particle moving in inversion-invariant potentials and magnetic field, let $\psi(\mathbf{r}, \sigma, t)$ be our wave function under inversion-self-similar knowledge Y . Then under inverted knowledge $\tilde{Y}\tilde{G}$ it is $\psi(-\mathbf{r}, \sigma, t)e^{i\alpha}$. But as it stays the same we have $\psi(-\mathbf{r}, \sigma, t)e^{i\alpha} = \psi(\mathbf{r}, \sigma, t)$ so $\psi(\mathbf{r}, \sigma, t)$ is an even or odd function of \mathbf{r} according as $e^{i\alpha}$ is $+1$ or -1 , i.e. according as the parity is even or odd.

3. Stationary states

When the inter-particle potential function, external potential fields and external magnetic field experienced by the particles of a quantum mechanical system are not dependent on the time (and we assume this throughout the present section) ‘stationary’ pure states of knowledge of the process are possible. The propositions that express a *stationary* pure state of knowledge make no reference to dynamical properties of the system belonging to *any particular time*.

Working in the (closed) sample space of all propositions about the motion in a certain time period let q denote the set of particle position coordinates and their z components of spin all relating to a fixed Cartesian coordinate system, and let $\psi(q, t)$ be our proper (or improper) wave function for any one stationary pure state of knowledge.

We apply the method of transformation groups (section 5.3 of Chapter I) to find the form of the time dependence of $\psi(q, t)$. Specifically we consider the effect of transforming the time variable by shifting the origin of the time by δ .

Letting $\tilde{\psi}(q, t)$ be our wave function in the new time coordinate we claim that under stationary conditions, the problem of finding the probability distribution $\tilde{\psi}(q, t)$ is *similar* to that of finding the probability distribution $\psi(q, t)$ in the original time coordinate. Accordingly, by (5.1.1)‡ of Chapter I, we have the functional relation

$$\tilde{\psi}(q, t) = \psi(q, t)e^{i\alpha}$$

where α is a real number independent of q and t , but possibly a function of δ . And by the uniqueness of probability assignments we also have the identity

$$\tilde{\psi}(q, t - \delta) = \psi(q, t)$$

* i.e. if they have the right kind of spatial symmetry

† This is simply because (as in section 2.2) our general knowledge G stays the same (with or without inversion) and so does our knowledge Y .

‡ where in the present case $Y^{(1)}G^{(1)} = Y^{(2)}G^{(2)} = YG$

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because $t - \delta$ on the LHS and t on the RHS refer to the same absolute time. And the last two equations hold for all q, t and δ . Combining them gives

$$\psi(q, t + \delta) = \psi(q, t)e^{i\alpha} \quad (3.1)$$

holding for all q, t and δ . Since wave functions are differentiable functions of their continuous variables, α is a differentiable function of δ and of course when $\delta = 0$, α must be zero also. Taking the case δ is an infinitesimal (3.1) gives for $\psi (= \psi(q, t))$

$$\frac{\partial \psi}{\partial t} \delta = \psi \cdot i\alpha'_0 \delta$$

where α'_0 is $\partial\alpha/\partial\delta$ at $\delta = 0$. Cancelling the δ s and solving the differential equation gives

$$\psi(q, t) = \psi(q, 0)e^{-iEt/\hbar} \quad (3.2)$$

where α'_0 has been written as $-E/\hbar$. So (3.2) is the general form of the time dependence of $\psi(q, t)$, E being a real constant with the units of energy which we will soon show is a property of the quantum mechanical process in question.

Now $\psi(q, t)$ must also satisfy the Schrödinger equation (e.g. in the case of a single spin zero particle it must satisfy (4.2.4) of Chapter IV, or in the case of pure spinning motion of a spin one-half particle it must satisfy (8.2.3) of Chapter VII). In general the Schrödinger equation has the form

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = \hat{H}\psi \quad (3.3)$$

where \hat{H} is the Hamiltonian operator always Hermitian and here assumed to be independent of the time. Substitution of (3.2) into (3.3) shows that therefore $\psi(q, t)$ has the form $\psi(q, t) = \phi(q)e^{-iEt/\hbar}$ with $\phi(q)$ satisfying the equation $\hat{H}\phi = E\phi$. Under requirements of symmetry (in the case some of the particles of the system are identical) and under boundary conditions imposed by physical constraints, this equation always has orthogonal solutions $\phi(q) = \phi_{nl}(q)$ with corresponding real eigenvalues E_n of E . As is well known, the functions $\phi_{nl}(q)$ form a complete set in that any wave function for the system can be expressed as a linear combination of them, and the general wave function of a *stationary* state can be written

$$\psi(q, t) = \phi_{nl}(q)e^{-iE_n t/\hbar} \quad (3.4)$$

where the $\phi_{nl}(q)$ are normalised thus*

$$\int \phi_{nl}^*(q)\phi_{n'l'}(q)dq = \delta_{nn'}\delta_{ll'} \quad (3.5)$$

and satisfy

$$\hat{H}\phi_{nl} = E_n\phi_{nl} \quad (3.6)$$

E_n being a monotonic increasing function of n , with n and l standing for one (in the case of n) and one or more (in the case of l) real, constant, dimensionless (discrete or continuous) parameters that serve to label all the possible stationary pure states of knowledge we may hold of the system. In any case where the particles of the system are confined to a finite region of space, the parameters n and l are all discrete.

Because the stationary state wave functions (3.4) form a complete set of orthogonal functions of q that are essentially time-independent (the time appearing only in the unimportant (q -independent) phase factor, it follows, from the law of inferred dynamical properties (section 3.12 of Chapter I) that there is an associated timeless property P_{nl} quantified by the parameters nl . A stationary state of knowledge of the dynamics of a system therefore amounts to knowledge of a property of the system quantified by a definite value of nl . This involves knowledge of the ‘energy’ E_n of the system which being a function of nl is itself a property going with the property represented by nl . Energy is thus a property present in all systems.†

If our wave function $\psi(q,t)$ at time t under *any* pure state of knowledge Y of the system dynamics is expanded in the wave functions (3.4) thus‡

$$\psi(q,t) = \sum_{nl} a_{nl}\phi_{nl}(q)e^{-iE_n t/\hbar} \quad (3.7)$$

the squared moduli of the coefficients a_{nl} , which must satisfy

* The notation in (3.5) and elsewhere is of course symbolic in that the integral may need to a multiple integral or a combination of integrals and sums and the Kronecker deltas might have to be delta functions etc.

† Even if a system’s Hamiltonian \hat{H} is a function of time equation (3.6) can still be employed to establish the existence of a set of orthogonal functions ϕ_{nl} at any one time t and hence a time dependent inferred dynamical property $P_{nl}(t)$ and an associated energy $E_n(t)$.

‡ Strictly speaking, since the set of possible l values depends on n we should write any sum $\sum_{nl} S_{nl}$ as $\sum_n (\sum_l S_{nl})$ because the sums over l and n are not reversible. And of course a sum may become an integral in the case n and/or l are continuously variable parameters.

$$\sum_{nl} |a_{nl}|^2 = 1, \quad (3.8)$$

are (as shown in section 6.3 of Chapter II) our degrees of belief that the property parameters take particular values n and l . Although the general wave function in (3.7) does not represent a stationary state of knowledge, the a_{nl} must nonetheless remain constant in time on account of (3.6) and the need for $\psi(q,t)$ to satisfy the Schrödinger equation (3.3). We may relate the a_{nl} to the pseudo wave function (under pure knowledge Y) over the pseudo basis P_{nl} (where the P_{nl} are the propositions claiming the properties P_{nl}), i.e. we can put

$$a_{nl} = \Phi(P_{nl}|Y)e^{i\alpha_{nl}}. \quad (3.9)$$

where α_{nl} are constant indeterminate phases (cf. equation before (6.3.4) of Chapter II). And if $P_{nl}t$ claims P_{nl} is present at time t we naturally claim

$$P_{nl}t \stackrel{0}{\Leftrightarrow} P_{nl}0 \quad (3.10)$$

for the property P_{nl} is timeless. By (3.10) the values of n and l stay constant in time and do so regardless of any knowledge we may hold about the motion.

But we cannot claim that the property P_{nl} quantified by nl is a *basic* property and that the functions $\phi_{nl}(q)$ are the transformation functions from P_{nl} to q . For after normalisation, equation (3.6) only fixes the $\phi_{nl}(q)$ to within a phase factor $e^{i\beta_{nl}}$ where β_{nl} may be an arbitrary real function of n and l .*

3.1 Stationary states of a particle moving under the influence of a time independent scalar potential

In this case the differential equation (3.6) for functions $\phi_{nl}(\mathbf{r})$ of particle position \mathbf{r} takes the form

$$-\frac{\hbar^2}{2m} \nabla^2 \phi_{nl} + V(\mathbf{r})\phi_{nl} = E_n \phi_{nl}, \quad (3.1.1)$$

where m is the mass of the particle. After normalisation, $\phi_{nl}(\mathbf{r})$ contains an unknown phase factor $e^{i\beta_{nl}}$.

* If we wanted to claim the $\phi_{nl}(q)$ were transformation functions we would have to determine the function β_{nl} at least to within an indeterminate additive real constant. It is not clear how this can be done.

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In some cases (i.e. for some $V(\mathbf{r})$), we will claim that the property P_{nl} is one that does not change under *time reversal*. Then since $V(\mathbf{r})$ is independent of the time and no vector potential is present, our knowledge YG is the same as its time reversed form $\tilde{Y}\tilde{G}$. Accordingly each wave function $\phi_{nl}e^{-iE_n t/\hbar}$ must remain the same under time reversal, i.e.

$$\phi_{nl}(\mathbf{r})e^{-iE_n t/\hbar} = (\phi_{nl}(\mathbf{r})e^{-iE_n(-t)/\hbar})^*$$

implying that the $\phi_{nl}(\mathbf{r})$ are all *real* functions of \mathbf{r} . Then only real solutions to (3.1.1) are needed and the (real) $\phi_{nl}(\mathbf{r})$ no longer contain arbitrary phase factors $e^{i\beta_{nl}}$. They still however have indeterminate signs (i.e. they contain indeterminate factors ± 1) possibly different for different values of nl . So if we were to try to claim that the P_{nl} represent a *basic* property and that the $\phi_{nl}(\mathbf{r})$ are the transformation functions from nl to \mathbf{r} , we would still need to determine (i.e. to somehow derive) the sign of each of the $\phi_{nl}(\mathbf{r})$ or at least the *relative* signs of them. So far we know no way of doing this so we refrain from claiming that the P_{nl} represent a basic property.

3.1.1 Particle in a box

Taking $V(\mathbf{r})$ infinite outside a box and zero within it, taking Cartesian coordinates with origin O at a vertex of the box and positive axes containing edges of the box, and leaving aside the arbitrary phase factor $e^{i\beta_{n_1 n_2 n_3}}$, (3.1.1) has the well-known solution

$$\phi_{n_1 n_2 n_3}(x, y, z) = \sqrt{\frac{8}{abc}} \sin \frac{n_1 \pi x}{a} \sin \frac{n_2 \pi y}{b} \sin \frac{n_3 \pi z}{c} \quad (3.1.1.1)$$

for \mathbf{r} lying inside the box, i.e. for $0 < x < a$, $0 < y < b$ and $0 < z < c$, and

$$\phi_{n_1 n_2 n_3}(x, y, z) = 0$$

for \mathbf{r} lying outside the box. In (3.1.1.1) n_1, n_2 and n_3 are numbers each taking the possible values $1, 2, \dots, \infty$. The possible stationary state wave functions are accordingly

$$\phi_{n_1 n_2 n_3}(x, y, z) e^{-iE_{n_1 n_2 n_3} t/\hbar} \quad (3.1.1.2)$$

where, by (3.1.1), the possible (kinetic) energy values are*

* The relation between the parameters $n_1 n_2 n_3$ and the parameters nl in the general form (3.4) of a stationary state is difficult to formulate. We would have to put in order the (distinct) energy values in (3.1.1.3) and label them n (with say $n = 1, 2, \dots, \infty$) and then distinguish parameter values $n_1 n_2 n_3$ that

$$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right). \quad (3.1.1.3)$$

We now assume $n_1 n_2 n_3$ represents a property invariant under time reversal. Then, as shown above, the $\phi_{n_1 n_2 n_3}$ are necessarily real and only the signs of the $\phi_{n_1 n_2 n_3}$ remain indeterminate. They are chosen *conventionally* to be all positive as in (3.1.1.1).

We note that the functions (3.1.1.1) (as is generally the case for eigenfunctions of the Hamiltonian) form a complete set of functions of x, y and z in so far as any allowed wave function (which, by continuity, must vanish at the inside surface of the box) can (by Fourier's theorem) be expanded in terms of them. They are orthonormal in the sense that

$$\int_0^c \int_0^b \int_0^a \phi_{n_1 n_2 n_3}(x, y, z) \phi_{n_1' n_2' n_3'}^*(x, y, z) dx dy dz = \delta_{n_1 n_1'} \delta_{n_2 n_2'} \delta_{n_3 n_3'}$$

From the form of (3.1.1.1) we see that our knowledge is separable into pure states of knowledge in the closed sample spaces S_x , S_y and S_z of all propositions concerning the components of the particle motion in the x, y and z directions respectively. Corresponding to (3.1.1.1) our wave function in S_x for example is

$$\phi_{n_1}(x, t) = \sqrt{\frac{2}{a}} \sin \frac{n_1 \pi x}{a} e^{-iE_{n_1} t / \hbar} \quad (3.1.1.4)$$

under the pure knowledge labelled by n_1 (taking values $1, 2, \dots, \infty$) and for which the component of kinetic energy in the x direction is

$$E_{n_1} = \frac{\pi^2 \hbar^2}{2m} \frac{n_1^2}{a^2}. \quad (3.1.1.5)$$

If we parallel displace the coordinates so the new origin O' is at the centre of the box, then relative to the new coordinates x', y' and z' we have

gave equal energies $E_{n_1 n_2 n_3}$ by a parameter l in some way. (True, in the special case a^{-2}, b^{-2} and c^{-2} were incommensurable, there would be no degeneracy and l would not be needed.) But rather than change the notation to the form nl it is easier to work with the new parameters n_1, n_2 and n_3 .

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$$\sin \frac{n_1 \pi x}{a} = \begin{cases} (-1)^{\frac{n_1-1}{2}} \cos \frac{n_1 \pi x'}{a} & n_1 \text{ odd} \\ (-1)^{\frac{n_1}{2}} \sin \frac{n_1 \pi x'}{a} & n_1 \text{ even} \end{cases} \quad (3.1.1.6)$$

and similarly for the other factors in (3.1.1.1).

Assuming knowledge $n_1 n_2 n_3$ is knowledge of a property that does not change on inversion through the centre of the box we see, from (3.1.1.6) and its equivalent for the y and z components, that the parity P of knowledge $n_1 n_2 n_3$ under such inversion is

$$P = \begin{cases} 1 & \text{for } n_1 + n_2 + n_3 \text{ odd} \\ -1 & \text{for } n_1 + n_2 + n_3 \text{ even} \end{cases}$$

i.e. the parity is even if $n_1 + n_2 + n_3$ is odd and odd if $n_1 + n_2 + n_3$ is even.

Let us now change to the momentum representation in the central coordinate system. Using the x component of the second of (5.1) of Chapter VI, our wave function in S_x (in the momentum representation) is

$$a'(p'_x, t) = a'(p'_x) e^{-iE_m t/\hbar} \quad (3.1.1.7)$$

where, dropping the primes, suffix x and suffix 1 for simplicity, we have by (3.1.1.6) and (3.1.1.4)

$$a'(p'_x) = a(p) = (2\pi\hbar)^{-1/2} \int_{-a/2}^{a/2} (-1)^{n/2} \sqrt{\frac{2}{a}} \begin{cases} -i \cos \frac{n\pi x}{a} \\ \sin \frac{n\pi x}{a} \end{cases} \exp(-ipx/\hbar) dx \quad \begin{cases} n \text{ odd} \\ n \text{ even} \end{cases}$$

where the function $(-1)^{n/2}$ is defined as in Appendix A (so that $(-1)^{1/2} = i$). Expanding the exponential into trig functions and dropping the odd part of the integral (which vanishes) we see we can let

$$\begin{cases} -i \cos \frac{n\pi x}{a} \\ \sin \frac{n\pi x}{a} \end{cases} \exp(-ipx/\hbar) \rightarrow -i \begin{cases} \cos \frac{n\pi x}{a} \cos \frac{px}{\hbar} \\ \sin \frac{n\pi x}{a} \sin \frac{px}{\hbar} \end{cases} = -\frac{1}{2} i \left(\cos\left(\frac{p}{\hbar} - \frac{n\pi}{a}\right)x \pm \cos\left(\frac{p}{\hbar} + \frac{n\pi}{a}\right)x \right) \quad \begin{cases} n \text{ odd} \\ n \text{ even} \end{cases}$$

where, on the RHS, 'odd' or 'even' refer to the \pm sign. And performing the integration we find

$$a(p) = (2\pi\hbar)^{-1/2} (-1)^{n/2} \sqrt{\frac{2}{a}} (-i) \left(\frac{\sin\left(\frac{p}{\hbar} - \frac{n\pi}{a}\right)\frac{a}{2}}{\frac{p}{\hbar} - \frac{n\pi}{a}} \pm \frac{\sin\left(\frac{p}{\hbar} + \frac{n\pi}{a}\right)\frac{a}{2}}{\frac{p}{\hbar} + \frac{n\pi}{a}} \right) \quad \begin{cases} n \text{ odd} \\ n \text{ even} \end{cases} \quad (3.1.1.8)$$

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where for n odd $(-1)^{n/2}(-i)$ is more conveniently written as $(-1)^{(n-1)/2}$. From (3.1.1.8) and (3.1.1.7), the momentum wave functions $a'(p'_x, t)$, $a'(p'_y, t)$ and $a'(p'_z, t)$ are easily constructed.

The possibility of periodic motion.

Consider motion of the particle in the box, when our pure knowledge Y of its motion is separable into pure knowledge of the components of motion in the x , y and z directions. Our general wave function relating to the x component of the motion is a function $\psi(x, t)$. This can be expanded in the stationary state wave functions (3.1.1.4) thus

$$\psi(x, t) = \sum_{n=1}^{\infty} a_n \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} e^{-iE_n t/\hbar} \quad (3.1.1.9)$$

where

$$E_n = \frac{\pi^2 \hbar^2}{2m} \frac{n^2}{a^2}. \quad (3.1.1.10)$$

and the a_n are independent of the time. The form (3.1.1.9) ensures $\psi(x, t)$ satisfies the 1-D Schrödinger equation. Now let Y be the knowledge that the particle is at $\mathbf{r} = \mathbf{r}_0$ at $t = 0$, so that $\psi(\mathbf{r}, 0) = \delta(\mathbf{r} - \mathbf{r}_0)$ or equivalently $\psi(x, 0) = \delta(x - x_0)$, $\psi(y, 0) = \delta(y - y_0)$ and $\psi(z, 0) = \delta(z - z_0)$ where x_0 is the x component of \mathbf{r}_0 etc.

At time $t = T$ where

$$T = \frac{4ma^2}{\pi\hbar} \quad (3.1.1.11)$$

we have, by (3.1.1.10), that $E_n t/\hbar = 2\pi n^2$ so the factor $e^{-iE_n t/\hbar}$ in (3.1.1.9) starts as 1 at $t = 0$ and returns to 1 at $t = T$. As a result $\psi(x, T) = \psi(x, 0) = \delta(x - x_0)$ and clearly

$$\psi(x, NT) = \delta(x - x_0) \quad (3.1.1.12)$$

for any integer N . This shows the x component of motion is *periodic* with period T . For (3.1.1.12) means that the proposition ‘the particle x coordinate is x_0 at time $t = 0$ ’ implies the proposition ‘the particle x coordinate is x_0 at time $t = NT$ ’ with a determinate phase of implication (namely zero). And since the origin of the time and the choice of x_0 in the range $0 < x_0 < a$ is arbitrary, the x component of free particle motion in a box is *naturally* periodic with period T given by (3.1.1.11). That is, it is periodic

regardless of any knowledge we may or may not have regarding the x component of motion (in addition to our knowledge that $0 < x < a$).

The three-dimensional motion of a particle in a box is therefore naturally periodic with period T if (and only if) multiples of the periods

$$T_1 = \frac{4ma^2}{\pi\hbar}, T_2 = \frac{4mb^2}{\pi\hbar} \text{ and } T_3 = \frac{4mc^2}{\pi\hbar}$$

of the x, y and z components of motion are equal, i.e. if (and only if)

$$N_1 T_1 = N_2 T_2 = N_3 T_3 = T$$

where N_1, N_2 and N_3 are the smallest positive integers that produce the equality. This requires that $N_1 a^2 = N_2 b^2 = N_3 c^2$ or

$$a^2 : b^2 : c^2 = N_1 : N_2 : N_3,$$

i.e. that the squares of the sides are in integral proportions. Then we find, from (3.1.1.3), that

$$\frac{E_{n_1 n_2 n_3} T}{\hbar} = 2\pi(N_1 n_1^2 + N_2 n_2^2 + N_3 n_3^2)$$

and accordingly any wave function

$$\psi(x, y, z, t) = \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{\infty} \sum_{n_3=1}^{\infty} a_{n_1 n_2 n_3} \sqrt{\frac{8}{abc}} \sin \frac{n_1 \pi x}{a} \sin \frac{n_2 \pi x}{a} \sin \frac{n_3 \pi x}{a} e^{-iE_{n_1 n_2 n_3} t / \hbar} \quad (3.1.1.13)$$

where the $a_{n_1 n_2 n_3}$ are arbitrary constants, is periodic with period T .

Since the motion is continuous and the particle does not move infinitely fast, its periodic motion during the time T must be motion along a closed path inside the box that leaves most of the box interior ‘unvisited’. We know little about the form of the path. It must be generally different each time the particle is prepared in a way that gives us a pure state of knowledge of its motion. (For example it must be generally different each time the ground state of stationary motion is prepared.) Otherwise there would be regions in which the particle was never found contrary to experience. In fact, under any pure knowledge, the wave function in any chosen 3-D region of the box interior is never zero at all times.*

* That the wave function may be zero in a 3-D region of the box at time $t = 0$, cease to be zero just after and be zero again at time $t = T$ shows that the Schrödinger equation governing the complex-valued probability distribution over the position of a particle differs greatly from the diffusion equation governing

3.1.2 Particle in a centrally symmetric field

With $V(\mathbf{r})$ equal to a function $U(r)$ of the distance r of the particle from the origin of fixed coordinates, equation (3.1.1) has the well-known solution which, with an arbitrary phase factor included, takes the form

$$\phi_{klm} = R_{kl}(r)\Phi_m(\phi)\Theta_{lm}(\theta)e^{i\beta_{klm}} \quad (3.1.2.1)$$

where r, θ and ϕ are the spherical polar coordinates of particle position,

$$\Phi_m(\phi) = (2\pi)^{-1/2} e^{im\phi}, \quad (3.1.2.2)$$

$$\Theta_{lm}(\theta) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{2(l+m)!}} P_l^m(\cos\theta) \quad (3.1.2.3)$$

and (real-valued) $R_{kl}(r)$ satisfies the ordinary differential equation

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR_{kl}}{dr} \right) - \frac{l(l+1)}{r^2} R_{kl} + \frac{2\mu}{\hbar^2} (E_{kl} - U(r)) R_{kl} = 0 \quad (3.1.2.4)$$

μ being the mass of the particle and E_{kl} the energy going with the property P_{klm} associated with the complete set of wave functions $\phi_{klm} e^{-iE_{kl}t/\hbar}$. The possible energies are independent of m and for continuity of the wave functions the parameters l and m are limited to the integer values

$$\begin{aligned} l &= 0, 1, 2, \dots, \infty \\ m &= -l, -l+1, \dots, l \end{aligned} \quad (3.1.2.5)$$

(The above results are derived for example in [12].*) As is well known the functions $\Phi_m(\phi)$ and $\Theta_{lm}(\theta)$ form complete sets of functions of ϕ and θ respectively which are orthonormal in the sense that

the (classical) probability distribution over the position of a (classical) particle in Brownian motion despite the fact that the mathematical derivations of the equations are formally similar (as shown in Appendix H).

* The equation (3.1.2.3) differs from (28.5) in [12] in that a factor i^l is omitted. The 'associated Legendre function' in (3.1.2.3) is defined as in the Mathematical Appendix §c of [12] i.e. as

$P_l^m(\cos\theta) = \sin^m \theta d^m P_l(\cos\theta) / (d \cos\theta)^m$ for $0 < m \leq l$ and $P_l^0(\cos\theta) = P_l(\cos\theta)$ where the Legendre polynomials are $P_l(x) = (2^l l!)^{-1} (d^l / dx^l) (x^2 - 1)^l$ with $P_0(x) = 1$, and

$P_l^{-m} = (-1)^m ((l-m)! / (l+m)!) P_l^m$ for $-l \leq m \leq l$.

$$\int_0^{2\pi} \Phi_m(\phi) \Phi_{m'}^*(\phi) d\phi = \delta_{mm'} \quad (3.1.2.6)$$

$$\int_0^\pi \Theta_{lm}(\theta) \Theta_{l'm'}^*(\theta) \sin \theta d\theta = \delta_{mm'} \delta_{ll'} \quad (3.1.2.7)$$

For any potential $U(r)$, suitable (normalised) solutions to (3.1.2.4) can be derived (as for example in (3.1.2.11) below) together with the possible eigenvalues of the energy E_{kl} and then the functions ϕ_{klm} given by (3.1.2.1) always form a complete set of orthonormal functions of r, θ and ϕ .

The energy is then a known function of klm . And as well as the energy E_{kl} we speak of $\sqrt{l(l+1)}$ being the ‘angular momentum’ of the particle with respect to the origin of coordinates and of m being the ‘component of angular momentum’ in the z direction. Both are measured in units of \hbar so the actual physical values are $\hbar\sqrt{l(l+1)}$ and $m\hbar$ respectively.

By (3.10), the properties of energy, angular momentum and its z component are all constants of the motion, i.e. all constant during any motion the particle may undergo in the central field. And this is true no matter what knowledge we may or may not hold about that motion.

We claim that under time reversal the energy and angular momentum remain the same and the z component of angular momentum changes sign. Therefore the problem of finding the wave function $\phi_{klm} e^{-iE_{kl}t/\hbar}$ under knowledge klm is *similar* to that of finding the wave function $\phi_{kl-m} e^{-iE_{kl}t/\hbar}$ under knowledge $kl-m$ and accordingly we require, by (1.1.2), that

$$\phi_{kl-m} e^{-iE_{kl}t/\hbar} = (\phi_{klm} e^{-iE_{kl}(-t)/\hbar})^*$$

or $\phi_{kl-m} = \phi_{klm}^*$ which is fulfilled by (3.1.2.1) and (3.1.2.2) (since $\Theta_{lm}(\theta)$ and $R_{kl}(r)$ are real, and $\Phi_{-m}(\phi) = \Phi_m^*(\phi)$) provided only that we make the phases β_{klm} in the phase factor $e^{i\beta_{klm}}$ antisymmetric in m , i.e. provided

$$\beta_{kl-m} = -\beta_{klm}.$$

The values of the β_{klm} are otherwise arbitrary but may, if we wish, be fixed by convention.

We also claim that any of the stationary states of knowledge is knowledge of a property that stays the same on inversion through the origin of coordinates. Accordingly the parity of our stationary state knowledge is $+1$ or -1 according as the wave function $\phi_{klm} e^{-iE_{kl}t/\hbar}$ is an even or odd function under the change of coordinates:

$$(r, \theta, \phi) \rightarrow (r, \pi - \theta, \phi + \pi).$$

Since $U(r)$ in (3.1.2.4) stays the same on inversion, $R_{kl}(r)$ stays the same, while, by (3.1.2.2)

$$\Phi_m(\phi) \rightarrow \Phi_m(\phi + \pi) = e^{im\pi} \Phi_m(\phi) = (-1)^m \Phi_m(\phi).$$

By (3.1.2.3), in which $\cos\theta \rightarrow \cos(\pi - \theta) = -\cos\theta$ and $P_l^m(\cos\theta) \rightarrow (-1)^{m+l} P_l^m(\cos\theta)^*$ we have

$$\Theta_{lm}(\theta) \rightarrow (-1)^{m+l} \Theta_{lm}(\theta).$$

As a result the parity of the general stationary state of knowledge is $(-1)^l$.

Case of a particle in a spherical cavity

When

$$U(r) = \begin{cases} 0 & 0 \leq r < a \\ \infty & r \geq a \end{cases} \quad (3.1.2.8)$$

the particle is restricted to move within a spherical cavity of radius a . The energy of the particle can only be kinetic energy which we assume is necessarily positive or zero. Hence $E_{kl} \geq 0$ and equation (3.1.2.4) becomes

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR_{kl}}{dr} \right) - \left(\frac{l(l+1)}{r^2} - K^2 \right) R_{kl} = 0$$

where

$$K = \frac{\sqrt{2\mu E_{kl}}}{\hbar} \quad (3.1.2.9)$$

and the (real) solution finite for $r \rightarrow 0$ is

$$R_{kl} = A_{kl} \sqrt{\frac{\pi}{2Kr}} J_{l+\frac{1}{2}}(Kr) \quad (3.1.2.10)$$

* This is because $\sin\theta \rightarrow \sin\theta$ while $P_l(\cos\theta) \rightarrow P_l(-\cos\theta) = (-1)^l P_l(\cos\theta)$ and $d^m/(d\cos\theta)^m \rightarrow (-1)^m d^m/(d\cos\theta)^m$. See previous footnote.

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where the A_{kl} are real numerical constants and $J_{l+\frac{1}{2}}$ are Bessel functions of fractional order (see p.437 of [21]).

The boundary condition that the wave function must (for continuity) vanish at $r = a$ gives the equation

$$J_{l+\frac{1}{2}}(Ka) = 0$$

for the possible values of K and hence E_{kl} . We may choose the k label as an integer $0,1,2,\dots,\infty$ standing for the $(k+1)^{\text{th}}$ positive zero $j_{l+\frac{1}{2},k+1}$ of the function $J_{l+\frac{1}{2}}(x)$ along the x axis. The lowest value of E_{kl} (the ground state) then occurs when $k=l=0$ corresponding to the first zero of $J_{\frac{1}{2}}(x)$ which is at $x = j_{\frac{1}{2},1} = 3.141593$ (see p.467 of [21] for the zeros of $J_{l+\frac{1}{2}}(x)$ for $x > 0$, $l = 0,1,2,\dots$). We therefore write $R_{kl}(r)$ as

$$R_{kl}(r) = A_{kl} \sqrt{\frac{\pi}{2Kr}} J_{l+\frac{1}{2}}\left(j_{l+\frac{1}{2},k+1} \frac{r}{a}\right) \quad (3.1.2.11)$$

where

$$K = j_{l+\frac{1}{2},k+1} \frac{1}{a} \quad (3.1.2.12)$$

and therefore, by (3.1.2.9), the (all different) energy levels are

$$E_{kl} = \frac{\hbar^2}{2\mu a^2} j_{l+\frac{1}{2},k+1}^2. \quad (3.1.2.13)$$

The $R_{kl}(r)$ must be normalised so that the ϕ_{klm} in (3.1.2.1) are orthonormal; i.e. so the ϕ_{klm} satisfy

$$\int_0^{2\pi} \int_0^\pi \int_0^a \phi_{klm} \phi_{k'l'm'}^* r^2 \sin \theta dr d\theta d\phi = \delta_{kk'} \delta_{ll'} \delta_{mm'}. \quad (3.1.2.14)$$

This requires

$$A_{kl}^2 \frac{\pi}{2} \int_0^1 \frac{1}{Kta} J_{l+\frac{1}{2}}\left(j_{l+\frac{1}{2},k+1} t\right) J_{l+\frac{1}{2}}\left(j_{l+\frac{1}{2},k'+1} t\right) (at)^2 a dt = \delta_{kk'}$$

giving, by 11.4.5 of [21],

$$A_{kl} = \frac{2}{a} \sqrt{\frac{K}{\pi}} (J'_{l+\frac{1}{2}}(j_{l+\frac{1}{2},k+1}))^{-1} \quad (3.1.2.15)$$

where the prime stands for the first derivative of the Bessel function with respect to its argument and the indeterminate sign is (by convention) taken to be +1 for all kl .

4. Quasi-static variation of a stationary state

Of special interest in quantum statistical mechanics is the manner in which the wave function (initially representing a stationary state of knowledge of a system) changes when a parameter of the Hamiltonian is changed very slowly to a new value. The parameter in question, which we will denote as a , is a parameter referring to an external potential to which the particles of the system are subjected. It is a parameter under our control and our knowledge of the system can, strictly speaking, remain stationary only when it is held constant.*

The following theory of quasi-static parameter variation is based on the account given in p.409-414 of [22].

For a *fixed* value of a our stationary state wave function must be of the general form (3.4) or, to make the a dependence explicit, of the general form

$$\psi(q,t) = \phi_{nl}(q,a) e^{-iE_n(a)t/\hbar} \quad (4.1)$$

where $\phi_{nl}(q,a)$ is an eigenfunction of the Hamiltonian $\hat{H}(a)$:

$$\hat{H}(a)\phi_{nl}(q,a) = E_n(a)\phi_{nl}(q,a) \quad (4.2)$$

and the eigenvalues E_n are functions of a (and for each value of a remain monotonic increasing functions of n). The indeterminate phase factors $e^{i\beta_{nl}(a)}$ in $\phi_{nl}(q,a)$ are supposed chosen in some conventional way so the $\phi_{nl}(q,a)$ are definite functions.

Now if the parameter a is varied by us in a controlled way, it becomes a known function $a(t)$ of t and our wave function $\psi(q,t)$ under any pure knowledge of the system will have to satisfy the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi(q,t)}{\partial t} = \hat{H}(a(t))\psi(q,t). \quad (4.3)$$

* An example of a parameter would be the length of one side of a box in which a particle moved freely (as in section 3.1.1); this length could be slowly varied but our knowledge of the particle motion could, strictly speaking be stationary only when it was held constant.

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Since the $\phi_{nl}(q, a)$, for all possible values of nl , form a complete set of orthogonal functions for any fixed value of a it is possible to expand $\psi(q, t)$ thus

$$\psi(q, t) = \sum_{nl} C_{nl}(t) \phi_{nl}(q, a) \quad (4.4)$$

where the $C_{nl}(t)$ are suitable functions of the time t , and we take a to equal $a(t)$ so a too is a function of time t in (4.4). Substituting this in (4.3) gives, on account of (4.2)

$$-\frac{\hbar}{i} \frac{\partial}{\partial t} \sum_{nl} C_{nl} \phi_{nl}(q, a) = \sum_{nl} C_{nl} E_n(a) \phi_{nl}(q, a).$$

When applied to functions of a , $\partial/\partial t$ is the same as $\dot{a} \partial/\partial a$ so this becomes

$$-\frac{\hbar}{i} \sum_{nl} \dot{C}_{nl} \phi_{nl}(q, a) - \dot{a} \frac{\hbar}{i} \sum_{nl} C_{nl} \frac{\partial \phi_{nl}(q, a)}{\partial a} = \sum_{nl} C_{nl} E_n(a) \phi_{nl}(q, a).$$

Changing nl to $n'l'$, multiplying through by $\phi_{n'l'}^*(q, a)$ and integrating over q the orthonormality of the $\phi_{nl}(q, a)$, which holds for any value of a , gives us the differential equation

$$-\frac{\hbar}{i} \dot{C}_{n'l'} = -\dot{a} \frac{\hbar}{i} \sum_{n'l''} C_{n'l''} \int \phi_{n'l''}^*(q, a) \frac{\partial \phi_{n'l'}(q, a)}{\partial a} dq + C_{n'l'} E_n(a) \quad (4.5)$$

for the time variation of the C_{nl} in (4.4).

Now if the rate of change of a is small enough the first term on the RHS of (4.5) will be negligible and the C_{nl} will change at least initially according to

$$-\frac{\hbar}{i} \dot{C}_{n'l'} = C_{n'l'} E_n(a) \quad (4.6)$$

which has the simple solution

$$C_{nl} = C_{nl}|_{t=0} e^{-\frac{i}{\hbar} \int_0^t E_n(a(t)) dt} \quad (4.7)$$

where only the phases of the C_{nl} are changing. In particular if we start out at $t=0$ with wave function $\psi(q, 0) = \phi_{nl}(q, a_0)$ (so $C_{n'l'}|_{t=0} = \delta_{nn'} \delta_{ll'}$) and make a slow change in a from a_0 at time $t=0$ to a at time t , (4.7) means our wave function $\psi(q, t)$ given by (4.4) is

$$\psi(q, t) = \phi_{nl}(q, a(t)) e^{-\frac{i}{\hbar} \int_0^t E_n(a(t)) dt} \quad (4.8)$$

reducing to (4.1) if there is no change in a from time $t=0$ to time t . Result (4.8) means our wave function remains the same apart from its natural dependence on a and the presence of a certain time dependent phase factor independent of the coordinates q .

However to ensure the truth of (4.7) and (4.8) we must take account of the fact that although \dot{a} is small in (4.5), it is present for a long time T during which a substantial change in a may occur. Formally we must consider the case when

$$\dot{a} \rightarrow 0 \text{ and } T \rightarrow \infty \quad (4.9)$$

while

$$\int_0^T \dot{a} dt = a(T) - a(0) \quad (4.10)$$

remains constant and is not necessarily small. It then seems possible that (4.5) will in the end lead to a change in the *amplitudes* of the C_{nl} as well as a change in their phases and that C_{nl} values that start out zero for some nl may, in the course of time, become non-zero. To show this is in fact not the case and that (4.7) and (4.8) can hold quite generally under the required conditions (4.9) and (4.10) (apart from a need to change the phase factor in (4.8)), we start by rewriting the governing equations (4.5) in terms of the variable a rather than t . So long as $a(t)$ is a monotonic function this is quite possible and we find that regarded as functions of a (not t) the equations for the C_{nl} are

$$-\frac{\hbar}{i} \frac{\partial C_{nl}}{\partial a} = -\frac{\hbar}{i} \sum_{n'l'} C_{n'l'} \int \phi_{nl}^* \frac{\partial \phi_{n'l'}}{\partial a} dq + \frac{1}{\dot{a}} C_{nl} E_n \quad (4.11)$$

to be satisfied for $a_0 \leq a \leq a_1$ where $a_0 = a(t)|_{t=0}$ and $a_1 = a(t)|_{t=T}$. In (4.11) C_{nl} , \dot{a} , E_n and the integral are all taken to be functions of a rather than t and the domain $a_0 \leq a \leq a_1$ is now fixed and finite. Supposing \dot{a} is small for all a between a_0 and a_1 the last term in (4.11) dominates suggesting the solution

$$C_{nl} = C_{nl}|_{a=a_0} e^{-\frac{i}{\hbar} \int_{a_0}^a \frac{1}{\dot{a}} E_n da} \quad (4.12)$$

equivalent to (4.7). But for generality we seek the solution of (4.11) in the general form

$$C_{nl} = F_{nl}(a) e^{-\frac{i}{\hbar} \int_{a_0}^a \frac{1}{\dot{a}} E_n da} \quad (4.13)$$

where the $F_{nl}(a)$ need not be (and are not) explicitly dependent on \dot{a} . Then (4.11) gives for $F_{nl}(a)$ the equation

$$-\frac{\hbar}{i} \frac{\partial F_{nl}}{\partial a} = \frac{\hbar}{i} \sum_{n'l'} F_{n'l'} e^{\frac{i}{\hbar} \int_{a_0}^a (E_n - E_{n'}) da} \int \phi_{nl}^* \frac{\partial \phi_{n'l'}}{\partial a} dq.$$

Integrating this gives

$$F_{nl}(a) - F_{nl}(a_0) = - \sum_{n'l'} \int_{a_0}^a F_{n'l'} e^{\frac{i}{\hbar} \int_{a_0}^a (E_n - E_{n'}) da} \left(\int \phi_{nl}^* \frac{\partial \phi_{n'l'}}{\partial a} dq \right) da. \quad (4.14)$$

We now show that the RHS of (4.14) may be taken to tend to zero as $\dot{a} \rightarrow 0$ for all a between a_0 and a_1 . Then (4.13) reduces to (4.12) confirming (4.7) and (4.8).

Firstly, the summand on the RHS of (4.14) clearly tends to zero as $\dot{a} \rightarrow 0$ provided $n \neq n'$. For then (since E_n is, for any a , a monotonic increasing function of n) the difference $E_n - E_{n'}$ is not zero for any a in the range $a_0 \leq a \leq a_1$, so $(E_n - E_{n'})/\dot{a}$ becomes larger and larger making the phase factor

$$e^{\frac{i}{\hbar} \int_{a_0}^a (E_n - E_{n'}) da}$$

a more and more rapidly fluctuating function of a reducing the main integral over a in (4.14) to zero.

Secondly, the summand term for which $n'l' = nl$ can be made to vanish even though $E_n - E_{n'}$ is then zero so no rapid fluctuation of the main integrand in (4.14) occurs. This can be done by choosing the constant phase factors allowed in the $\phi_{nl}(q, a)$ so that

$$\int \phi_{nl}^* \frac{\partial \phi_{nl}}{\partial a} dq = 0. \quad (4.15)$$

For by the normality of the ϕ_{nl} we have

$$\frac{\partial}{\partial a} \int \phi_{nl}^* \phi_{nl} dq = 0$$

so

$$\int \phi_{nl}^* \frac{\partial \phi_{nl}}{\partial a} dq = - \left[\int \phi_{nl}^* \frac{\partial \phi_{nl}}{\partial a} dq \right]^*$$

or

$$\int \phi_{nl}^* \frac{\partial \phi_{nl}}{\partial a} dq = ip_{nl}(a)$$

where $p_{nl}(a)$ is a real function of a . So if (4.15) is not already satisfied we change from the ϕ_{nl} to the Φ_{nl} defined by

$$\Phi_{nl}(q, a) = \phi_{nl}(q, a) e^{-i \int_{a_0}^a p_{nl}(a) da} \quad (4.16)$$

and then (4.15) will be satisfied, i.e. we will have

$$\int \Phi_{nl}^* \frac{\partial \Phi_{nl}}{\partial a} dq = 0. \quad (4.17)$$

This is easily confirmed by substituting (4.16) into (4.17). So by adopting an appropriate choice for the variation with a of the previously mentioned (coordinate independent) phase factors $\beta_{nl}(a)$ in the $\phi_{nl}(q, a)$ we can arrange that (4.15) is satisfied by the ϕ_{nl} . (By (4.16) the constant phase factors in the wave functions $\phi_{nl}(q, a_0)$ at time $t=0$ are unaffected and may still satisfy any constraints that might be imposed by knowledge other than our knowledge of the variation of a which is redundant as far as $\phi_{nl}(q, a_0)$ is concerned.)

Thirdly, the remaining summand terms in (4.14), i.e. those for which $n'=n$ but $l' \neq l$ vanish because

$$\int \phi_{nl}^* \frac{\partial \phi_{nl'}}{\partial a} dq = 0$$

for any unequal values of l and l' . This is because of the orthogonality of the eigenfunctions ϕ_{nl} that share the same energy, i.e. because

$$\int \phi_{nl}^* \phi_{nl'} dq = 0, \quad l \neq l'$$

and because differentiation of the factor $\phi_{nl'}$ in the integrand with respect to a does not change the orthogonal property. A general proof of the last claim is missing but its truth

XI. Time reversal, parity and stationary states

is evidently not at all affected by whether or not a phase factor $\exp(-i \int_{a_0}^a p_{nl}(a) da)$ has to be included in $\phi_{nl}(q, a)$, and it seems to be always true. For example, in the case of quasi-static variation of the stationary states of a particle in a box where the side of dimension a is slowly changed (while dimensions b and c remain constant) it follows from (3.1.1.3) that for certain triplets n_1, n_2, n_3 sharing the same value of n_1 the energies say $E_{n_1 n_2 n_3}$ and $E_{n_1 n'_2 n'_3}$ may be equal (for all a) because it may happen that

$$\frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} = \frac{n_2'^2}{b^2} + \frac{n_3'^2}{c^2}.$$

But in that case we will certainly have (with $\phi_{n_1 n_2 n_3}(x, y, z)$ as in (3.1.1.1)) that

$$\int_0^c \int_0^b \int_0^a \phi_{n_1 n_2 n_3}^* \frac{\partial}{\partial a} \phi_{n_1 n'_2 n'_3} dx dy dz = 0.$$

This easily follows from the product rule of differentiation and the orthogonality of trig functions (as in Fourier series). Similarly, in the case of quasi-static stationary states of a particle in a spherical cavity (section 3.1.2) with the radius of the cavity slowly changed

$$E_{kl} = E_{k'l'}$$

for any radius a of the cavity when klm and $k'l'm'$ differ only in regard to the values of m and m' . But

$$\int_0^{2\pi} \int_0^\pi \int_0^a \phi_{klm}^* \frac{\partial}{\partial a} \phi_{k'l'm'} r^2 \sin \theta dr d\theta d\phi = 0$$

when $kl = k'l'$ and $m \neq m'$, as easily follows from the orthogonality relation (3.1.2.6) and the fact that only $R_{kl}(r)$ in (3.1.2.1) depends on a .

In conclusion it seems always true that a quasi-static variation of a parameter a in the Hamiltonian leaves a stationary state wave function unchanged except for a phase factor independent of the coordinates q of the system. If our initial wave function is

$$\Psi(q, t)|_{t=0} = \phi_{nl}(q, a_0) \quad (4.18)$$

then after quasi-static variation of a from a_0 to some value $a(t)$ at time t it becomes

$$\Psi(q, t) = \phi_{nl}(q, a(t)) e^{-\frac{i}{\hbar} \int_0^t E_n(a(t)) dt - \int_{a_0}^{a(t)} i p_{nl}(a) da} \quad (4.19)$$

where (as in (4.2)) $\phi_{nl}(q, a)$ is an eigenfunction of $\hat{H}(a)$ the constant phase factor in which is fixed (for different values of a) by convention in any way we choose, $E_n(a)$ is the corresponding energy and

$$ip_{nl}(a) = \int \phi_{nl}^*(q, a) \frac{\partial \phi_{nl}(q, a)}{\partial a} dq, \quad (4.20)$$

$p_{nl}(a)$ being necessarily real. The parameters nl thus remain constant during quasi-static variation of a , the probability of any other values $n'l'$ of the parameters at any time t being zero. But of course the physical quantities quantified by nl generally change because of their dependence on a . The phase factor in the wave function (4.19) reflects the peculiar manner of expressing our knowledge that leads to this wave function, i.e. the knowledge that the parameter a is quasi-statically changed from its initial value a_0 at time $t=0$ to its value $a(t)$ at time t .

CHAPTER XII

APPROACHING THE CLASSICAL LIMIT

In other branches of modern physics (in special relativity for example) the conditions under which the classical limit is approached can be established directly from the physical laws (from the relativistic laws in the case of special relativity). But in the case of quantum mechanics this is not possible because we do not know the detailed quantum mechanical laws of motion. Instead we need to claim that under certain specified states of knowledge of a quantum mechanical process the orbital motion of the particles proceeds (to classical accuracy) as it would in classical mechanics, i.e. the representation point in configuration space moves (to classical accuracy) along one or other of a set of specifiable classical paths* and a certain classical probability can be assigned to each of these paths.

According to the correspondence principle (section 3.4 of Chapter III) we may have a *pure* state of knowledge of a quantum mechanical process under which the particles in question move in an approximately classical manner and more and more precisely so in a certain limit. We call such pure states of knowledge ‘quasi-classical’ and we refer to the corresponding wave functions as ‘quasi-classical wave functions’. Then in the limit the modulus squared of the wave function over any property with classical analogue (the position of a particle or the momenta of a particle etc.) averaged over vanishingly small domains if necessary) gives the classical probability distribution we should hold for that property when interpreting our knowledge of the process in a classical manner. Each such distribution demonstratively changes in time in a way consistent with particle motion in classical orbits. We thus claim that quasi-classical states of knowledge are both pure states of knowledge of quantum mechanical motions *and*, in the limiting case, ordinary states of knowledge of the classical motions that the particles are expected to follow.

1. Quasi-classical wave functions for a single particle

1.1 The Hamilton-Jacobi equation

We first note that in classical mechanics a *set* of possible motions of a particle under the action of potentials $V(\mathbf{r}, t)$ and $A(\mathbf{r}, t)$ can be associated with a classical action function

* The acquisition of any one of the specified states of knowledge generally interferes with the process physically (on account of the uncertainty principle) and this brings about or ensures that the representation point moves (to classical accuracy) along one or other of a set of classical orbits.

$S(\mathbf{r}, t)$ (a function of position \mathbf{r} and time t) which is a solution of the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S - \mathbf{A})^2 + V = 0. \quad (1.1.1)$$

Having found a solution to this equation we define a set of particle motions by stipulating that at every point \mathbf{r} and time t there is a particle with velocity

$$\mathbf{v} = \frac{1}{m}(\nabla S - \mathbf{A}). \quad (1.1.2)$$

We then have many copies of our particle of mass m moving together as a swarm of particles throughout the region of space and time in which $S(\mathbf{r}, t)$ is specified. If we follow any one of the particles in its motion we can confirm that it does move classically. For the acceleration of it is

$$\frac{d\mathbf{v}}{dt} = \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v}$$

and the force on it is therefore

$$\mathbf{F} = m \frac{d\mathbf{v}}{dt} = m \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} \right).$$

Since $(\mathbf{v} \cdot \nabla)\mathbf{v} = \frac{1}{2} \nabla(v^2) - \mathbf{v} \times (\nabla \times \mathbf{v})$ equations (1.1.1) and (1.1.2) give

$$\mathbf{F} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla V + \mathbf{v} \times (\nabla \times \mathbf{A})$$

which is just as it should be (see end of section 1 of Chapter III).

1.2 The simplest quasi-classical wave function

In the closed sample space of all propositions concerning the orbital motion of the particle over a time period t_0 to t_1 the quasi-classical wave function over particle position and of the simplest kind is one of the form

$$\psi(\mathbf{r}, t) = a(\mathbf{r}, t)e^{iS(\mathbf{r}, t)/\hbar} \quad (1.2.1)$$

where a and S are real valued functions with certain properties to be described. Inserting (1.2.1) into the Schrödinger equation 4.2.4 of Chapter IV with $\alpha, \gamma, \epsilon, \beta$ given their known values $\frac{1}{2}, -1, 1, 0$, we see that a and S must satisfy

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S - \mathbf{A})^2 + V - \frac{\hbar^2}{2m} \frac{\nabla^2 a}{a} = 0, \quad (1.2.2)$$

$$\frac{\partial a^2}{\partial t} + \nabla \cdot (a^2 \frac{\nabla S - \mathbf{A}}{m}) = 0. \quad (1.2.3)$$

We now assert that wave function (1.2.1) (which, as it stands, is of course quite a general function of \mathbf{r} and t) has a quasi-classical form whenever (i) V, \mathbf{A}, a and S are changing relatively slowly with \mathbf{r} and t (i.e. changing only over values of \mathbf{r} and t considered to be classical distances and times), (ii) \mathbf{A} is not too large*, (iii) $|S/\hbar| \gg 1$ (so the phase is very rapidly changing with the values of \mathbf{r} and t), and (iv) the fourth term in (1.2.2) is negligible to the degree that

$$\frac{\sqrt{|\hbar^2 \nabla^2 a/a|}}{\sqrt{(\nabla S - \mathbf{A})^2}} \ll 1. \quad (1.2.4)$$

Then (1.2.2) is the same as the Hamilton-Jacobi equation.

We assert that under the above conditions the particle moves (to classical accuracy) on one of the classical trajectories specified by $S(\mathbf{r}, t)$ in the manner of section 1.1, and that the classical probability for it being in one or other of the trajectories passing through any classical volume element $d^3\mathbf{r}$ at time t is $a^2(\mathbf{r}, t)d^3\mathbf{r}$ where \mathbf{r} is the position of $d^3\mathbf{r}$.

The above assertion is consistent with the necessary classical probability continuity equation

$$\frac{\partial a^2}{\partial t} + \nabla \cdot (a^2 \mathbf{v}) = 0 \quad (1.2.5)$$

because (1.2.5) is a consequence of (1.2.3) and (1.1.2).

The case of motion in a definite orbit

The form (1.2.1) under the conditions (i)-(iv) stated above can be a quasi-classical wave function for motion in a *definite* classical orbit. This is the case when a is of significant

* For example, a classical particle with a charge e and momentum \mathbf{p} may move, in a uniform magnetic field \mathbf{H} , in a circular orbit of radius p/H . If \mathbf{H} is too large, i.e. if its vector potential $\mathbf{A} (= e\mathbf{A}_{em}/c)$ is too large, the radius of the orbit will be too small to be considered a classical dimension.

value only within a classically infinitesimal (moving) region ΔV of space and, while S takes values both within and outside of ΔV , $\nabla S - \mathbf{A}$ is (to classical accuracy) constant within ΔV . Then the momentum as well as the position of the particle is definite to classical accuracy at each moment in time.

If Δ_r is the characteristic dimension of ΔV (and therefore of a) we require, from (1.1.2) and (1.2.4) that

$$\frac{\hbar/\Delta_r}{mv} \ll 1$$

i.e. that

$$mv \gg \hbar/\Delta_r. \quad (1.2.6)$$

We suppose that during the time period t_0 to t_1 our wave function is and remains a minimal wave packet in both position and momentum space. That is we suppose at all times that

$$\Delta_r \Delta_p \approx \hbar \quad (1.2.7)$$

where Δ_p is the uncertainty in the momentum. Then we see from (1.2.6) that the particle kinetic momentum mv is always large compared with Δ_p .

It is known that a solution of the Hamilton-Jacobi equation can always be found that includes any one specified classical orbit (see for example p.41 of [14]). Therefore a quasi-classical wave packet function of the form (1.2.1) always exists to represent classical motion on any one specified classical orbit. Of course, during its motion, such a wave packet expands on account of the quantum mechanical uncertainty in the initial particle momentum. Even though this uncertainty is (classically) ‘infinitesimal’ it still, in the course of time, threatens to convert the ‘infinitesimal’ Δ_r into a non-infinitesimal. The initial uncertainty in momentum is Δ_p and in time t from the beginning of the time period considered the resulting wave packet expansion is of order $\Delta_p t/m$. This should not be large compared to Δ_r , so we require

$$t \lesssim \frac{m\Delta_r}{\Delta_p}. \quad (1.2.8)$$

This imposes a limit (arising from quantum mechanics) on the concept of motion ‘in a definite orbit’ or on the time period $t_1 - t_0$ during which such motion can be expected to occur. The particle may still move a fairly long way under the condition (1.2.8). For in a time of order $m\Delta_r/\Delta_p$ it moves a distance of order $vm\Delta_r/\Delta_p$ or $(mv/\Delta_p)\Delta_r$ which is large compared to Δ_r .

The case of extended wave packets

As well as the ‘minimal’ wave packet form of a quasi-classical wave function representing motion in a definite orbit we have the ‘extended’ wave packet form. Here conditions (i)-(iv) of section 1.2 are still supposed to hold but the spacial dimension $\tilde{\Delta}_r$ of the wave packet and the range $\tilde{\Delta}_p$ of particle momentum now represent *classical* uncertainties in position and momentum. In place of (1.2.7) we must now have

$$\tilde{\Delta}_r \tilde{\Delta}_p \gg \hbar \quad (1.2.9)$$

and, $\tilde{\Delta}_r$ and $\tilde{\Delta}_p$ are no longer classical ‘infinitesimals’.

The extended wave packet can be classically quite confined (and the momentum range quite small) but not so small that we have motion in a definite orbit. Rather we expect to have classical motion in one or other of a bundle of classical orbits fairly close to one another with a certain classical probability associated with each. The spreading of such a packet is expected (and is explicable classically) and poses no limit to the time period considered.

The extended wave packet can alternatively be spread more widely. It can for example take the form of an expanding spherical wave packet of wide radial thickness giving a (classical) probability distribution over (classical) uniform rectilinear particle motions in one or other direction away from (and after scattering by) a centre of force.

Whatever the form of the extended wave packet it must be such that conditions (i)-(iv) of section 1.2 are met and consequently $S(\mathbf{r}, t)$ in (1.2.1) satisfies (1.1.1). This restricts the possible classical orbits to one or other of a set represented by a solution of the Hamilton-Jacobi equation. Therefore not every possible set of classical orbits can be represented by a quasi-classical wave function of the simplest kind. To represent *any* set of classical orbits by quasi-classical wave functions of the simplest kind superpositions of them are required.

1.3 Superpositions of quasi-classical wave functions of the simplest kind

We now claim that any number of normalised quasi-classical wave functions of the simplest kind may be sometimes superimposed (linearly combined) to represent another quasi-classical state of knowledge. (We take as an example two normalised quasi-classical (spin-less) single particle wave functions $\psi_1(\mathbf{r}, t)$ and $\psi_2(\mathbf{r}, t)$.) The result is a quasi-classical wave function $\psi(\mathbf{r}, t)$ of the form

$$\psi(\mathbf{r}, t) = k_1 \psi_1(\mathbf{r}, t) + k_2 \psi_2(\mathbf{r}, t) \quad (1.3.1)$$

where k_1 and k_2 are (generally complex) constants consistent with $\psi(\mathbf{r}, t)$ being normalised. However the combination $\psi(\mathbf{r}, t)$ is only quasi-classical at times in which

the separate wave functions ($\psi_1(\mathbf{r}, t)$ and $\psi_2(\mathbf{r}, t)$) do not ‘seriously interfere’, i.e. when the modulus squared of $\psi(\mathbf{r}, t)$ averaged over classically infinitesimal regions of space is effectively given by

$$\overline{|\psi(\mathbf{r}, t)|^2} = |k_1|^2 \overline{|\psi_1(\mathbf{r}, t)|^2} + |k_2|^2 \overline{|\psi_2(\mathbf{r}, t)|^2} \quad (1.3.2)$$

the bar representing the result of the averaging. In the absence of ‘serious interference’ the cross terms $(k_1\psi_1(\mathbf{r}, t))^* k_2\psi_2(\mathbf{r}, t)$ and $k_1\psi_1(\mathbf{r}, t)(k_2\psi_2(\mathbf{r}, t))^*$ that should generally be included in (1.3.2) are either exceedingly small or very rapidly alternating in space so that they average to something exceedingly small.

The absence of ‘serious interference’ requires that when they cross, the waves in the wave packets $\psi_1(\mathbf{r}, t)$ and $\psi_2(\mathbf{r}, t)$ are nowhere waves of equal or nearly equal (vector) wave number so that constructive or destructive interference or ‘beating’ over classical distances is avoided. The waves in $\psi_1(\mathbf{r}, t)$ and $\psi_2(\mathbf{r}, t)$ should therefore have quite different wavelengths, or, if they have the same wavelengths, they should travel in opposite directions or cross one another at an angle that is not too shallow.

At times in which the combination (1.3.1) is quasi-classical we clearly have

$$|k_1|^2 + |k_2|^2 = 1 \quad (1.3.3)$$

and we claim the following law:

Law of superposition of quasi-classical wave functions

The particle moves (to classical accuracy) either on one of the classical orbits associated with $\psi_1(\mathbf{r}, t)$ or on one of the classical orbits associated with $\psi_2(\mathbf{r}, t)$.

The classical probability for it being in one of the first set of trajectories is $|k_1|^2$ times the classical probability that would apply to that trajectory under the quasi-classical wave function $\psi_1(\mathbf{r}, t)$, and the classical probability for it being in one of the second set of trajectories is $|k_2|^2$ times the classical probability that would apply to that trajectory under the quasi-classical wave function $\psi_2(\mathbf{r}, t)$.*

As an example we consider the (often discussed) case of a particle passing through an interferometer (Figure 1.3.1). Let our pure state of knowledge be represented by an

* This law generalises naturally to many particle systems where the representation point in configuration space is expected to move in one or other of a number of classical trajectories associated with quasi-classical wave packets moving in that space.

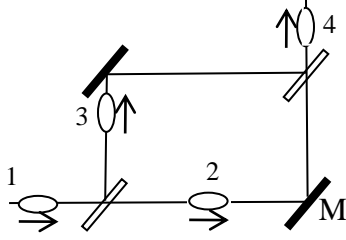


Figure 1.3.1

extended monochromatic wave packet 1 approaching the first (half-silvered) mirror*. This mirror, being at 45° to the path of the packet, causes the packet to split into two packets 2 and 3 moving along two separate arms of the interferometer. These packets are perfectly reflected into the other two arms of the interferometer and arrive together at the second half-silvered mirror where, on passing through it, we suppose they interfere *destructively* to zero on one exit path and interfere *constructively* on the other.

After splitting of the wave packet by the first half-silvered mirror at time t_1 and before reaching the final half-silvered mirror at time t_2 the wave function in this example is a quasi-classical superposition of two extended wave packets. However, during passage through the second half-silvered mirror ‘serious interference’ takes place so the quasi-classical nature of our knowledge does not apply to the motion at this time. After passage through the second half-silvered mirror when only wave packet 4 is present the quasi-classical nature of our knowledge of the motion is present again. Of course our pure state of knowledge of the actual (quantum mechanical) motion applies throughout and is represented by the total wave function.

From the time t_1 when the wave packets leave the first half-silvered mirror to the time t_2 just before they arrive at the second, our wave function $\psi(\mathbf{r}, t)$ is the superposition

$$\psi(\mathbf{r}, t) = \frac{1}{\sqrt{2}} \psi_1(\mathbf{r}, t) + \frac{1}{\sqrt{2}} \psi_2(\mathbf{r}, t) \quad (1.3.4)$$

where $\psi_1(\mathbf{r}, t)$ and $\psi_2(\mathbf{r}, t)$ are separate (normalised) quasi-classical extended wave packets moving along the two arms of the interferometer. By our general law of superposition the wave function $\psi(\mathbf{r}, t)$ is quasi-classical over this period of time. And it follows that (to classical accuracy) the particle either moves in one or other of the orbits associated with $\psi_1(\mathbf{r}, t)$, or in one or other of the orbits associated with $\psi_2(\mathbf{r}, t)$, and that it moves (with equal classical probability) either along one arm of the interferometer or along the other. However this is certainly not the same as claiming that either wave function $\psi_1(\mathbf{r}, t)$ or wave function $\psi_2(\mathbf{r}, t)$ should apply with equal classical probability.

* The ‘mirrors’ of the interferometer can of course be modelled as potential barriers, infinitely high for perfect reflection and of a finite height for partial reflection. By a ‘monochromatic’ wave packet we mean one representing knowledge which includes very precise knowledge of the particle momentum (to classical accuracy). The wave packet is extended but classically confined so that its dimension is large compared to the de Broglie wavelength but small compared to the size of the mirrors.

That would amount to claiming we are in a (non-pure) *mixed state* of knowledge contrary to hypothesis and if this was so we would not predict the interference that is certainly present after passage through the second half-silvered mirror.

It is however true that between times t_1 and t_2 , and when working to *classical accuracy*, our *classical* probability distribution should be either $|\psi_1(\mathbf{r}, t)|^2$ or $|\psi_2(\mathbf{r}, t)|^2$ with a *classical* probability $\frac{1}{2}$ for each case.* When working only to classical accuracy in this time period it is perfectly possible (in any trial) to determine which way the particle went after leaving the first half-silvered mirror without affecting the motion (i.e. the time dependence of properties with a classical analogue from time t_1 to time t_2) in any way that could be considered significant.

As we have said before, acquisition of knowledge is not problematical in classical physics and classical probability theory. It is problematical in quantum physics and complex-valued probability theory, and this is why the above claim that either wave function $\psi_1(\mathbf{r}, t)$ or wave function $\psi_2(\mathbf{r}, t)$ should apply is invalid. If we work to *quantum mechanical* accuracy and determine by *harmless conditioning* (i.e. by null measurement along one of the possible paths) that the pure state wave function $\psi_1(\mathbf{r}, t)$ should apply (to within an indeterminate phase factor) then the actual motion of the particle through the final half-silvered mirror is found to be different. The null-measurement (i.e. the external field employed to make it[†]) seems to influence the motion of the particle near time t_2 and this is strikingly revealed in the interferometer because (under the null detection) the particle may pass either way through the final half-silvered mirror.[‡]

But before reaching the final half-silvered mirror (and without any harmless conditioning), let us suppose the wave packets are reflected by new fully silvered mirrors

* As we have said, it is generally necessary to average the squared modulus of a quasi-classical wave function over classically small regions before we have the classical probability distribution. But in the case of simple non-overlapping monochromatic wave packets this is not necessary because the modulus of the wave function is already smoothly distributed over space.

[†] This might, for example, be a large potential gradient impulse applied at a time t ($t_1 < t < t_2$) to the region occupied by $\psi_1(\mathbf{r}, t)$, and designed to send the particle off at high speed (should it be in that region) to a particle detector.

[‡] The possible effect of the external field (employed in the null measurement) on the motion of the particle which might have passed through it (but did not) may appear mysterious. But note that it is not so different from the situation in the least action formulation of classical mechanics where the claim is made that the motion of a particle from point **A** at time t_1 to **B** at time t_2 is by the orbit that, of all possible orbits through the external potential field as a whole, is the one which minimises (or more generally represents a turning point in) the total action between times t_1 and t_2 . For in that formulation of classical mechanics the motion of the particle seems also to be affected by the potential along orbits the particle *might* have taken but did not. (We note in passing that a generalised principle of least action for classical mechanics could allow for the particle to take one or more of widely different orbits between fixed points **A** and **B** (each representing a local turning point of the action) with a probability assigned to each, calculated on the basis of Bayesian probability theory. In that case the potential field as a whole is also affecting our degrees of belief regarding which orbit the particle takes. For example, in a mirror symmetric potential field with just two possible particle orbits (one the mirror image of the other) the principle of indifference would lead us to assign (classical) probabilities of one-half to each orbit.)

and made to cross one another in perpendicular paths. As they cross, interference occurs and ‘fringes’ are present. But this is not ‘serious interference’ because it does not affect the value of the square of the modulus of the total wave function averaged over classically small volume elements. When viewed to *quantum mechanical accuracy* the interference is of course important.* But when viewed to classical accuracy it is not.

Note that in the original interferometer geometry there are interference fringes near either of the fully silvered mirrors where the approaching wave packet and its reflection overlap. These too are important when we work to quantum mechanical accuracy but not important when working to classical accuracy. This is a new kind of superposition because it is a superposition of one wave packet on *itself* (during reflection) and not a superposition of two separate wave packets. In this new kind of superposition the quasi-classical nature of the wave function still applies so long as the interference is again not ‘serious interference’.

1.4 Part-quasi-classical wave functions

Sometimes a wave function $\psi(\mathbf{r},t)$ demonstratively consists of the superposition of a quasi-classical wave function $\psi_{\text{qc}}(\mathbf{r},t)$ and a non-quasi-classical wave function $\psi_0(\mathbf{r},t)$, where $\psi_{\text{qc}}(\mathbf{r},t)$ and $\psi_0(\mathbf{r},t)$ are well separated in space and therefore essentially non-overlapping functions of position during the time period considered. Then we have

$$\psi(\mathbf{r},t) = k_0\psi_0(\mathbf{r},t) + k_{\text{qc}}\psi_{\text{qc}}(\mathbf{r},t) \quad (1.4.1)$$

where k_0 and k_{qc} are complex constants and $\psi_{\text{qc}}(\mathbf{r},t)$ and $\psi_0(\mathbf{r},t)$ are both normalised.

The constants k_0 and k_{qc} must clearly satisfy

$$|k_0|^2 + |k_{\text{qc}}|^2 = 1 \quad (1.4.2)$$

and we claim that under the pure state of knowledge represented by $\psi(\mathbf{r},t)$ and during the time period in question either the particle moves (to classical accuracy) in a classical manner in one or other of a set of classical orbits as if the wave function $\psi_{\text{qc}}(\mathbf{r},t)$ applied on its own, *or* the particle remains somewhere in the part of space in which $\psi_0(\mathbf{r},t)$ has significant absolute value. And the probabilities for one or the other possibility are $k_{\text{qc}}e^{i\alpha}$ and $k_0e^{i\beta}$ respectively where α and β are an indeterminate phases.†

* Measurements of particle position to quantum mechanical accuracy would show the particle avoids places in the fringes where the total wave function is zero.

† We stress that we are *not* supposing that one or other of the *wave functions* $\psi_{\text{qc}}(\mathbf{r},t)$ and $\psi_0(\mathbf{r},t)$ should apply. That would only be true after null detection of the particle in one or other of the separate regions of space occupied by $\psi_{\text{qc}}(\mathbf{r},t)$ and $\psi_0(\mathbf{r},t)$. In particular, if we observe no particle moving

We call this the *law of motion under a part-quasi-classical wave function**. It generalises naturally to many particle systems, and it applies in cases in which the quasi-classical part is a *superposition* of quasi-classical wave functions of the simplest kind. In the case of a single particle, each wave function in the superposition may include a factor of the form $\delta_{\sigma\sigma'}$ representing a definite (but generally different) z component of the particle's spin relative to a fixed Cartesian coordinate system.†

2. Quasi-classical stationary wave functions

The wave functions $\phi_{nl}(q)e^{-iE_n t/\hbar}$ of *stationary* states of knowledge (see section 3 of Chapter XI) become quasi-classical in the limit of large values of n and l .‡ We consider particular cases.

2.1 Case of a particle in a box

The stationary state wave functions in this case are given in section 3.1.1 of Chapter XI. We start by considering the form of the momentum distribution formula (3.1.1.8) of Chapter XI. With n large the two terms in the large bracket of that formula approach delta functions centred at $p = n\pi\hbar/a$ and $p = -n\pi\hbar/a$. For example, apart from a constant factor the first term in the large bracket is

$$\frac{\sin(p - p_0) \frac{a}{2\hbar}}{p - p_0} \tag{2.1.1}$$

where $p_0 = n\pi\hbar/a$. This peaks at $p = p_0$ which for large n is a momentum of classical magnitude. Because of the formal identity

$$\lim_{\alpha \rightarrow \infty} \frac{\sin p\alpha}{p} = \pi\delta(p)$$

(see Representation 2 in Appendix B) and the extreme smallness of \hbar in (2.1.1) we can set (2.1.1) equal to $\pi\delta(p - p_0)$.

Similar remarks apply to terms in the expression for $|a(p)|^2$. By (3.1.1.8) of Chapter XI

classically in regions where $\Psi_{qc}(\mathbf{r}, t)$ passes, we naturally claim our wave function should be changed from (1.4.1) to $\Psi_0(\mathbf{r}, t)$ times an indeterminate phase factor.

* This law will be needed in the modelling of measurements (Chapter XIII).

† See section 3 of Chapter XIII.

‡ This assumes of course appropriate ordering of n and l values.

$$|a(p)|^2 = (2\pi\hbar)^{-1} \frac{2}{a} \left(\frac{\sin^2(p-p_0) \frac{a}{2\hbar}}{(p-p_0)^2 \frac{1}{\hbar^2}} + \frac{\sin^2(p+p_0) \frac{a}{2\hbar}}{(p+p_0)^2 \frac{1}{\hbar^2}} \right) \quad (2.1.2)$$

where the cross term in the expansion of the square of the large bracket is for us negligible and therefore omitted. Formally in the limit as $\hbar \rightarrow 0$ (2.1.2) becomes

$$|a(p)|^2 = \frac{1}{2}(\delta(p-p_0) + \delta(p+p_0)) \quad (2.1.3)$$

on account of the identity

$$\lim_{\alpha \rightarrow \infty} \frac{\sin^2 p\alpha}{p^2\alpha} = \pi\delta(p)$$

(see Representation 3 in Appendix B).

Accordingly the momentum component p'_x of section 3.1.1 of Chapter XI, is for large n_1 expected to be close to $n_1\pi\hbar/a$ with likely error of order $\pi\hbar/a$. And for very large n_1, n_2 and n_3

$$p'_x \rightarrow \pm n_1\pi\hbar/a, \quad p'_y \rightarrow \pm n_2\pi\hbar/b, \quad p'_z \rightarrow \pm n_3\pi\hbar/c \quad (2.1.4)$$

or the absolute values of the components of momentum are expected to assume definite values to classical accuracy, the likely errors $\pi\hbar/a, \pi\hbar/b$ and $\pi\hbar/c$ (for classical box dimensions) being classically infinitesimal. The classical kinetic energy is $(p'^2_x + p'^2_y + p'^2_z)/2m$ so under (2.1.4) the quantum mechanical energy $E_{n_1n_2n_3}$ in (3.1.1.3) of Chapter XI coincides with the classical expression consistent with the momentum and kinetic energy being each quantum mechanical properties with a classical analogue.

In the classical limit, and only then, we see that n_1, n_2 and n_3 represent the properties of absolute value of the momentum components and our state of knowledge consists of knowledge of these absolute values. Given only such classical knowledge of the particle dynamics we deduce, by the principle of indifference of classical probability, that the particle is equally likely to be in any one of equal (classically) infinitesimal volume elements filling the box. That is, the classical probability density over particle *position* is $1/abc$ everywhere inside the box. This is in agreement with the form of the wave function (3.1.1.1) of Chapter XI, this wave function being now a quasi-classical wave function. Taking the modulus squared of this wave function we obtain

$$|\phi_{n_1n_2n_3}(x, y, z)|^2 = \frac{8}{abc} \sin^2 \frac{n_1\pi x}{a} \sin^2 \frac{n_2\pi y}{b} \sin^2 \frac{n_3\pi z}{c}$$

which (for large n_1, n_2 and n_3) becomes, on averaging over classically infinitesimal volume elements, exactly $1/abc$.

2.2 Case of a particle in a spherical cavity

We claim generally that the quantum mechanical property represented by parameters klm in section 3.1.2 of Chapter XI, namely the property of having simultaneously an angular momentum $L = \hbar\sqrt{l(l+1)}$ with respect to the origin of coordinates, a z component of angular momentum $M = m\hbar$, and an energy $E = E_{kl}$, is a property with classical analogue. When k, l and m are large compared with 1 the stationary state wave function $\phi_{klm}(r, \theta, \phi)$ of section 3.1.2 of Chapter XI becomes quasi-classical and L, M and E represent continuous classical properties.

Since there is no particle potential in the spherical cavity case, E is just the kinetic energy of the particle. And classically speaking, given just the values of L, M and E we should be able to deduce (using classical mechanics and classical probability theory) the probability density $p(r, \theta, \phi)$ over the particle position coordinates r, θ and ϕ inside the cavity. This probability density gives the probability $P(dV|LME)$ that the particle lies in volume element $dV = r^2 \sin \theta dr d\theta d\phi$ according to the formula

$$P(dV|LME) = p(r, \theta, \phi) r^2 \sin \theta dr d\theta d\phi. \quad (2.2.1)$$

And $p(r, \theta, \phi)$ should equal the modulus squared of $\phi_{klm}(r, \theta, \phi)$ averaged over (classically) infinitesimal volume elements if necessary. We deduce $p(r, \theta, \phi)$ as follows.

In the first place, given only L, M and E we are evidently indifferent with regard to the value of the coordinate ϕ of the particle, so

$$P(d\phi|LME) = g(\phi) d\phi$$

with

$$g(\phi) = \frac{1}{2\pi}.$$

Knowing dr and $d\theta$ would make no difference to the probability $P(d\phi|LME)$ and therefore $P(dr d\theta d\phi|LME) = P(dr d\theta|LME)P(d\phi|LME)$ and it remains to find $P(dr d\theta|LME)$.

Let L be the vector angular momentum of the particle pointing out from the origin of coordinates in a direction specified by spherical polar angles θ_L and ϕ_L . Then

$$M = L \cos \theta_L. \quad (2.2.2)$$

And as M and L are both given, so is θ_L . Now ϕ_L is unknown but assuming it given at one moment in time we have L at that time and hence know $r \times v$, v being the particle velocity and r its position. And r and v must be in a plane P through the origin and perpendicular to L .

In the plane P take polar coordinates (ρ, β) as follows. Let the polar coordinates share the same origin as our main coordinates and let the x axis of the polar coordinates (i.e. the line $\beta = 0$ or π) lie in the intersection of P with the xy plane of our main coordinates. And, as β increases (with ρ constant), let the point (ρ, β) move in circular motion left-handed with respect to the L direction. Given the radial coordinate ρ of the particle and the angular momentum angle ϕ_L we are clearly indifferent with regard to the value of its β coordinate, i.e.

$$P(d\beta|\rho\phi_L LME) = g(\beta)d\beta$$

where $g(\beta) = 1/2\pi$. Since the probability density $P(d\beta|\rho\phi_L LME)$ is independent of ρ and ϕ_L we can say that

$$P(d\beta|LME) = g(\beta)d\beta$$

with

$$g(\beta) = \frac{1}{2\pi}.$$

For given LME the θ coordinate of the particle depends on β but not on ρ or ϕ_L . Therefore the probability density $f(\theta)$ in

$$P(d\theta|LME) = f(\theta)d\theta$$

can be found from the dependence of θ on β . And since this distribution is independent of ρ and therefore of r , knowledge of dr would not change our probability $P(d\theta|LME)$ and therefore

$$P(dr d\theta|LME) = P(dr|LME)P(d\theta|LME)$$

Since the relation between θ and β is independent of ϕ_L we may suppose that $\phi_L = \pi$ and that the line $\beta = 0$, $0 < \rho < \infty$ lies along the positive y axis of our main coordinates. Taking a point (ρ, β) in P and calculating its z coordinate in two ways we obtain

$$z = \rho \cos \theta = \rho \sin \beta \sin \theta_L.$$

Hence

$$\sin \beta \sin \theta_L = \cos \theta \quad (2.2.3)$$

and as β ranges from $-\pi$ to π , the angle θ always satisfies

$$\begin{aligned} \frac{\pi}{2} - \theta_L < \theta < \frac{\pi}{2} + \theta_L, & \quad \text{if } 0 < \theta_L < \frac{\pi}{2} \\ \frac{\pi}{2} - (\pi - \theta_L) < \theta < \frac{\pi}{2} + (\pi - \theta_L), & \quad \text{if } \frac{\pi}{2} < \theta_L < \pi \end{aligned} \quad (2.2.4)$$

and the same value of θ occurs twice, once at say β and again at $\pi - \beta$. Hence the probability density $f(\theta)$ over θ is related to $g(\beta)$ by

$$f(\theta)|d\theta| = g(\beta)|d\beta| + g(\pi - \beta)|d\beta| = \frac{1}{\pi}|d\beta|$$

and using (2.2.3)

$$f(\theta) = \frac{1}{\pi} \left| \frac{d\beta}{d\theta} \right| = \frac{1}{\pi} \frac{\sin \theta}{|\cos \beta| \sin \theta_L} = \frac{1}{\pi} \frac{\sin \theta}{\sqrt{1 - \sin^2 \beta} \sin \theta_L}$$

which (again by (2.2.3)) becomes

$$f(\theta) = \frac{1}{\pi} \frac{\sin \theta}{\sqrt{\sin^2 \theta_L - \cos^2 \theta}} \quad (2.2.5)$$

and clearly $f(\theta) = 0$ for θ outside the limits given in (2.2.4).

As the particle is free it must move with constant velocity $v (= \sqrt{2E/\mu})$ in the plane P perfectly reflecting off the circular boundary C formed by the intersection of P and the cavity wall. The centre point of the chord along which the particle moves is a distance r_{LE} from the origin where

$$r_{LE} = \frac{L}{\mu v} = \frac{L}{\sqrt{2\mu E}} \quad (2.2.6)$$

and evidently

$$p(r, \theta, \phi) = 0 \quad 0 \leq r < r_{LE}. \quad (2.2.7)$$

And since r_{LE} cannot be greater than a there is a necessary limitation of parameter values:

$$\frac{L}{\sqrt{2\mu E}} < a. \quad (2.2.8)$$

As the particle moves along the chord C at constant velocity it is equally likely to be in any element ds of the chord length. Therefore the probability for the r coordinate of particle position to lie between r and $r + dr$ (for $r_{LE} < r < a$) is proportional to

$$ds = \frac{dr}{\sin \alpha}$$

where α is the angle between the perpendicular to the chord (let fall from the origin) and the radius vector of position of the element ds , so that $\sin \alpha = \sqrt{r^2 - r_{LE}^2} / r$. Therefore the probability distribution $h(r)$ over r for $r_{LE} < r < a$ is given by $h(r)dr = cds$ where c is some constant. That is

$$h(r) = \frac{c}{\sin \alpha} = \frac{cr}{\sqrt{r^2 - r_{LE}^2}} \quad (2.2.9)$$

and $h(r) = 0$ for $0 < r < r_{LE}$. For normalisation, the constant c has to be

$$c = \frac{1}{\sqrt{a^2 - r_{LE}^2}}. \quad (2.2.10)$$

We have found that the probability distributions over position coordinates r, θ and ϕ are logically independent, i.e.

$$P(dr d\theta d\phi | LME) = h(r)dr \cdot f(\theta)d\theta \cdot g(\phi)d\phi$$

where $g(\phi) = 1/2\pi$. Comparison with (2.2.1) (in which proposition dV is equivalent to proposition $dr d\theta d\phi$) gives

$$p(r, \theta, \phi) = \frac{h(r)}{r^2} \cdot \frac{f(\theta)}{\sin \theta} \cdot \frac{1}{2\pi} \quad (2.2.11)$$

or by (2.2.5) and (2.2.9)

$$p(r, \theta, \phi) = \frac{cr}{\sqrt{r^2 - r_{LE}^2}} \cdot \frac{1}{\pi} \frac{\sin \theta}{\sqrt{\sin^2 \theta_L - \cos^2 \theta}} \cdot \frac{1}{2\pi r^2 \sin \theta}$$

for

$$r_{LE} < r < a$$

$$\frac{\pi}{2} - \theta_L < \theta < \frac{\pi}{2} + \theta_L, \quad \text{if } 0 < \theta_L < \frac{\pi}{2} \quad \text{or}$$

$$\frac{\pi}{2} - (\pi - \theta_L) < \theta < \frac{\pi}{2} + (\pi - \theta_L), \quad \text{if } \frac{\pi}{2} < \theta_L < \pi$$

and zero for other values of r and θ .

To show the correspondence principle applies we have to show that for large k , l and m , the density $p(r, \theta, \phi)$ in (2.2.11) equals the modulus squared of the stationary state wave function $\phi_{klm}(r, \theta, \phi)$ (in the form (3.1.2.1) of Chapter XI) averaged over (classically) infinitesimal volume elements if necessary.

This will evidently be so if (with bars denoting the required averaging over classically infinitesimal elements dr or $d\theta$) we have

$$\begin{aligned} \overline{r^2 |R_{kl}(r)|^2} &= h(r), \\ \overline{\sin \theta |\Theta_{lm}(\theta)|^2} &= f(\theta), \\ |\Phi_m(\phi)|^2 &= g(\phi) = \frac{1}{2\pi}, \end{aligned} \tag{2.2.12}$$

where the functions $R_{kl}(r)$, $\Theta_{lm}(\theta)$ and $\Phi_m(\phi)$ are given by (3.1.2.10), (3.1.2.3) and (3.1.2.2) of Chapter XI, and $h(r)$ and $f(\theta)$ are given by (2.2.9) and (2.2.5).

The last equality in (2.2.12) is evidently satisfied on account of the simple form of $\Phi_m(\phi)$ in (3.1.2.2) of Chapter XI. For the other two equalities to hold we require, by (3.1.2.10) and (3.1.2.3) of Chapter XI, and taking $0 < \theta_L < \frac{\pi}{2}$, that for large k , l and m

$$\overline{r^2 A_{kl}^2 \frac{\pi}{2Kr} J_{l+\frac{1}{2}}^2(Kr)} = \begin{cases} cr / \sqrt{r^2 - r_{LE}^2} & r_{LE} < r < a \\ 0 & 0 < r < r_{LE} \end{cases} \tag{2.2.13}$$

and

$$\overline{\sin \theta \frac{(2l+1)(l-m)!}{2(l+m)!} (P_l^m(\cos \theta))^2} = \begin{cases} \sin \theta / (\pi \sqrt{\sin^2 \theta_L - \cos^2 \theta}) & \frac{\pi}{2} - \theta_L < \theta < \frac{\pi}{2} + \theta_L \\ 0 & 0 < \theta < \frac{\pi}{2} - \theta_L \\ 0 & \frac{\pi}{2} + \theta_L < \theta < \pi \end{cases} \dots \tag{2.2.14}$$

Expressions for A_{kl} and K are given in (3.1.2.15) and (3.1.2.12) of Chapter XI. Also r_{LE} is given by (2.2.6) with $L = \sqrt{l(l+1)}\hbar$ and E equal to the E_{kl} of (3.1.2.13) of Chapter XI. Hence

$$r_{LE} = \frac{\sqrt{l(l+1)}a}{j_{l+\frac{1}{2},k+1}} \quad (2.2.15)$$

and θ_L is given by (2.2.2) and is therefore

$$\theta_L = \cos^{-1} \frac{m}{\sqrt{l(l+1)}}. \quad (2.2.16)$$

The demonstration of the equalities (2.2.13) and (2.2.14) could doubtless be accomplished analytically. But we content ourselves here with numerical illustrations. For $k=12$ and $l=30$ the LHS and RHS of (2.2.13) (without averaging of the LHS) are plotted in Fig 2.2.1. And for $l=50$ and $m=40$ the LHS and RHS of (2.2.14) (without averaging of the LHS) are plotted in Fig 2.2.2. In both figures the dashed lines plot the RHS of the respective equation and the full lines the LHS (without averaging). Numerical experimentation with increasing values of k, l and m confirms that (except increasingly close to the boundaries $r = r_{LE}$ and $\theta = \frac{\pi}{2} \pm \theta_L$ of the classical distributions) the left hand sides of (2.2.13) and (2.2.14) (even before averaging) become extremely small at values of r and θ for which the *right hand sides* are zero, and within the boundaries of the classical distributions the left hand sides of (2.2.13) and (2.2.14) approach squared sine-wave-like forms of higher and higher frequency whose moving averages closely fit the corresponding classical probability distributions.

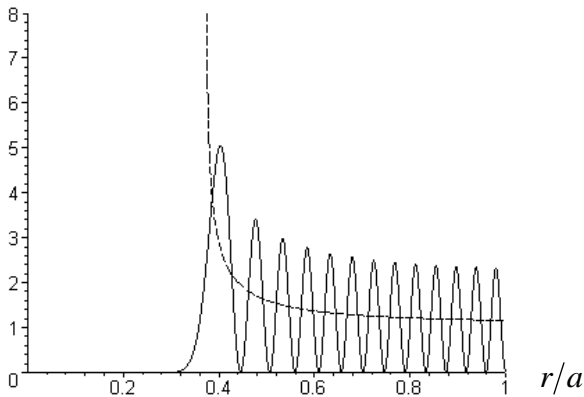


Figure 2.2.1

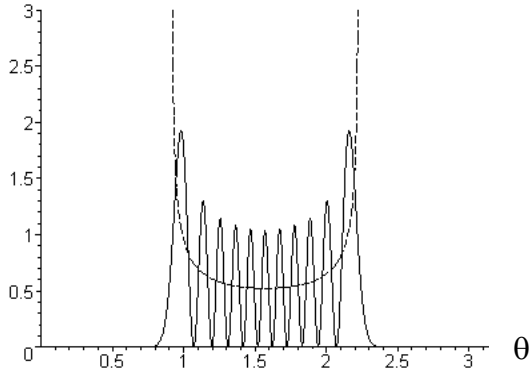


Figure 2.2.2

3. Generalisation

The theory (in section 1) of quasi-classical wave functions for the orbital motion of a single particle may be generalised in a natural manner to cover orbital motions of two or more particles some of which may be identical. As is well known the (classical) Hamilton-Jacobi theory applies in the configuration space of a many particle classical system. Accordingly the ‘simplest quasi-classical wave functions’ over such a space can be specified in an analogous way. So can superpositions of them. Physical properties and probabilities relating to part quasi-classical and part ordinary wave functions can also be claimed for many particle systems. And quasi-classical stationary state wave functions can be identified much as in the single particle case (section 2).

When the particles of a many particle system are expected to move classically (to classical accuracy) in separate classical orbits, the identical particles can be distinguished. And while their natural order remains of course unknown, we are at liberty to claim a natural order of them if we wish.

When we theorise about the combined orbital and spinning motions of a system of two or more particles any claim that they move classically can only be applied to their orbital motions because spin is not a property with classical analogue. A quasi-classical wave function of a system of particles with spin must therefore take account of this fact. To represent well defined classical orbital motions of each particle under an inter-particle potential, slowly varying external scalar and vector potentials and a uniform magnetic field, the wave function can be of the form of a product of two functions, a quasi-classical wave function over position coordinates (represented by a wave packet moving in configuration space) and an ordinary wave function over the z components of spin, the orbital and spinning motions then proceeding independently.* Extended wave packets and superpositions of wave packets are then possible with a classical interpretation (regarding the orbital motions) so long as the wave packets in configuration space do not ‘seriously interfere’.

* This can also apply (at least when there is no inter-particle potential) when the magnetic field is *non-uniform* and the particles are each expected to closely follow a definite classical orbit. The magnetic field experienced by each particle is then a known function of the time.

MODELLING THE ACQUISITION OF KNOWLEDGE

We now consider the modelling of *measurement* processes, processes by which we may acquire knowledge of various dynamical properties of quantum mechanical systems to quantum mechanical accuracy. We assume that the dynamical properties of particles moving in the classical limit (properties, that is, that have a classical analogue (like position and momentum)) are *directly* observable (to classical accuracy) and that we need not inquire into how the acquisition of knowledge of *these* properties is accomplished.

We will not generally be modelling *practical* measurement techniques. Instead we will attempt to model the simplest possible processes which *in principle* accomplish the measurements required.* The kit available for modelling measuring apparatus may consist, in short, of anything possible in principle in quantum mechanics. It therefore may consist of particles of any mass, charge and magnetic moment, and of inter-particle scalar potential functions of any number of different kinds depending on particle positions and the time in a variety of ways, some particles being susceptible to some kinds of inter-particle potential and others to others. Since different kinds of particles may, in quantum theory, occupy the same positions (whatever their spins), we are at liberty to construct background material filling all space yet having no effect on the quantum mechanical system under study. This background material can take the form of very many particles of high mass held closely together by inter-particle potentials to which the quantum mechanical systems under study are not susceptible. Since the masses of the particles can be as large as we please, such a structure can constitute classical material and serve as a coordinate system including synchronised clocks at every point if we wish.

We also assume we are at liberty to set up sources that can produce any external (generally time dependent) scalar and vector potential fields to which one or more kind of particle of a quantum mechanical system under study may be sensitive.† We assume sources themselves may penetrate the quantum mechanical systems under study without directly interfering with them.‡

In section 2 and onwards we present models of some measurement processes. These serve to confirm the possibility previously claimed of acquiring knowledge of certain dynamical properties of quantum mechanical systems in a way which is consistent

* Impractical but instructive demonstrations of the possibility of acquiring knowledge of physical variables are of course common in classical physics. In classical electrodynamics for example we may suppose that the electric field at every point in space could be measured to any degree of accuracy at any time. This could be done for instance by observing the momentary displacements of particles of vanishingly small mass and charge each fixed to one end of springs of vanishing mass, size and elasticity, the other ends of the springs being fixed to a rigid background material that does not interfere with the field etc. Clearly these conditions cannot be met in actual practice but *are* possible in principle.

† This resembles the assumption in classical mechanics that we are able to apply any (generally time dependent) force to any particle of a system under study.

‡ For example a macroscopic current density used to produce an external magnetic field may pass through a hydrogen atom under study without directly affecting it. See *Note on the relativistic modelling of electromagnetic field sources* in Appendix C.

with the laws of quantum mechanics and (complex-valued) probability theory. The cases covered are hopefully enough to convince us that we could model, and in principle carry out, any measurement assumed possible in theory.

First however (in section 1) we study the effects of certain impulsive actions on the wave function representing a pure state of knowledge of a particle's orbital motion. This study is of interest in itself but it will also enable the reader more easily to follow the work of section 2 onwards.

1. The effect of impulsive actions on a wave function

1.1 Case of a free particle

Consider the orbital motion of a free particle of mass m under pure knowledge Y represented by a wave function $\psi(\mathbf{r}, t)$, \mathbf{r} being the particle position in fixed coordinates. We suppose $\psi(\mathbf{r}, t)$ always falls fast enough to zero as $|\mathbf{r}| \rightarrow \infty$ so that we can claim to know the particle is, at any time t , within a certain fixed finite region W_t of space. (W_t is, we may say, the region occupied by $\psi(\mathbf{r}, t)$ at time t .) During a short time $t = a$ to $t = a + \delta$ let us apply an external scalar potential field V (to which the particle is sensitive) given by

$$V = -kx \quad (1.1.1)$$

over the whole region W_a .^{*} Here k is a real constant and x is the x coordinate of a point in W_a . We will consider the limit as $k \rightarrow \infty$ and $\delta \rightarrow 0$ while $k\delta$ remains finite.

The Schrödinger equation for $\psi(\mathbf{r}, t)$ during time $t = a$ to $t = a + \delta$ is

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi - kx\psi \quad (1.1.2)$$

but since $k \rightarrow \infty$ only the term $-kx\psi$ on the RHS matters. The solution of (1.1.2) is therefore

$$\psi(\mathbf{r}, t) = \psi(\mathbf{r}, a) e^{ikx(t-a)/\hbar} \quad a < t < a + \delta \quad (1.1.3)$$

and in the limit we see that $\psi(\mathbf{r}, a)$ is instantly changed to $\psi'(\mathbf{r}, a)$ given by^{*}

^{*} In the case the particle carries a charge, V could be an electric potential created by a surface charge density source and surface dipole (i.e. double layer) density source distributed over the boundary of W_a . The surface charge density would account for the discontinuity of the normal component of the electric field (from $-(\nabla V)_n$ to zero) and the surface dipole density would (independently) account for the discontinuity in V (from V to zero) across the boundary.

$$\psi'(\mathbf{r}, a) = \psi(\mathbf{r}, a)e^{ikx\delta/\hbar} \quad (1.1.4)$$

Let $a(\mathbf{p}, t)$ be the original (undisturbed) wave function $\psi(\mathbf{r}, t)$ in the momentum representation[†] so that

$$a(\mathbf{p}, a) = (2\pi\hbar)^{-3/2} \int_{W_a} \psi(\mathbf{r}, a)e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} d^3\mathbf{r}. \quad (1.1.5)$$

Let $a'(\mathbf{p}, t)$ be the momentum wave function going with $\psi'(\mathbf{r}, t)$ for $t > a$ so that

$$a'(\mathbf{p}, a) = (2\pi\hbar)^{-3/2} \int_{W_a} \psi'(\mathbf{r}, a)e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} d^3\mathbf{r} \quad (1.1.6)$$

Then by (1.1.4) – (1.1.6)

$$a'(\mathbf{p}, a) = a(\mathbf{p} - k\delta\hat{\mathbf{i}}, a) \quad (1.1.7)$$

where $\hat{\mathbf{i}}$ is the unit vector in the x direction. Hence $a'(\mathbf{p}, a)$ is the same as $a(\mathbf{p}, a)$ except for a boost $k\delta\hat{\mathbf{i}}$ in momentum.

After the impulse has acted (i.e. for $t > a$) the wave function $\psi(\mathbf{r}, t)$ has changed to

$$\psi'(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int a'(\mathbf{p}, a) \exp[i(\mathbf{p}\cdot\mathbf{r} - E(t-a))/\hbar] d^3\mathbf{p} \quad (1.1.8)$$

where $E = p^2/2m$. This is because (1.1.8) satisfies (1.1.2) (with $k=0$) and gives the correct expression for $\psi'(\mathbf{r}, t)$ (the inverse of (1.1.6)) when $t=a$. Substituting for $a'(\mathbf{p}, t)$ using (1.1.7) gives

$$\psi'(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int a(\mathbf{p} - k\delta\hat{\mathbf{i}}, a) \exp[i(\mathbf{p}\cdot\mathbf{r} - E(t-a))/\hbar] d^3\mathbf{p}.$$

Changing (in the integral) the origin of momentum space to $k\delta\hat{\mathbf{i}}$ this becomes

* Result (1.1.4) also follows from the general solution of the Schrödinger equation for a particle in a scalar potential of uniform gradient ((5.12) of Chapter VI). If we put (in (5.12) of Chapter VI) $\mathbf{v} = k\hat{\mathbf{i}}$ (where \mathbf{v} there represents the negative of the potential gradient) and $t = \delta$, and take the limit $k \rightarrow \infty$ and $\delta \rightarrow 0$ while $k\delta$ remains constant we confirm (1.1.4) in the case when $a = 0$. This shows (1.1.4) holds if (in (1.1.2)) x or ψ should (for isolated values of \mathbf{r} and t) vanish in W_a so that $-kx\psi$ would only *almost always* be the dominate term on the RHS of the Schrödinger equation.

[†] we should not of course confuse the a in $a(\mathbf{p}, t)$ with the time $t = a$

$$\psi'(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int a(\mathbf{p}, a) \exp i [((\mathbf{p} + k\hat{\delta}\mathbf{i})\mathbf{r} - E(\mathbf{p} + k\hat{\delta}\mathbf{i})(t-a)) / \hbar] d^3\mathbf{p}.$$

where

$$E(\mathbf{p} + k\hat{\delta}\mathbf{i}) = (\mathbf{p} + k\hat{\delta}\mathbf{i})^2 / 2m = (p^2 + k^2\delta^2 + 2\mathbf{p}\cdot\hat{\mathbf{i}}k\delta) / 2m.$$

Hence

$$\psi'(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} e^{i(k\hat{\delta}\mathbf{i}\cdot\mathbf{r} - k^2\delta^2(t-a)/2m)/\hbar} \int a(\mathbf{p}, a) \exp i [(\mathbf{p}\cdot(\mathbf{r} - k\hat{\delta}\mathbf{i}(t-a)/m) - E_0(t-a)) / \hbar] d^3\mathbf{p}$$

where $E_0 = p^2/2m$. Or since the undisturbed wave function $\psi(\mathbf{r}, t)$ is given by

$$\psi(\mathbf{r}, t) = (2\pi\hbar)^{-3/2} \int a(\mathbf{p}, a) \exp i [(\mathbf{p}\cdot\mathbf{r} - E_0(t-a)) / \hbar] d^3\mathbf{p}$$

(cf. (1.1.8)), we have

$$\psi'(\mathbf{r}, t) = e^{i(k\hat{\delta}\mathbf{i}\cdot\mathbf{r} - k^2\delta^2(t-a)/2m)/\hbar} \psi(\mathbf{r} - k\hat{\delta}\mathbf{i}(t-a)/m, t). \quad (1.1.9)$$

The wave function therefore evolves as it would have normally except that it is now being bodily propelled at velocity $k\hat{\delta}\mathbf{i}/m$ through space and phase modulated by the factor

$$e^{i(k\hat{\delta}\mathbf{i}\cdot\mathbf{r} - k^2\delta^2(t-a)/2m)/\hbar} = e^{ik^2\delta^2 a/2m\hbar} e^{i(k\hat{\delta}\mathbf{i}\cdot\mathbf{r} - k^2\delta^2 t)/2m\hbar}$$

which represents a constant phase factor $e^{ik^2\delta^2 a/2m\hbar}$ and a wave $e^{i(\boldsymbol{\kappa}\cdot\mathbf{r} - \omega t)}$ of unit amplitude with wave number $\boldsymbol{\kappa}$ and angular frequency ω given by

$$\boldsymbol{\kappa} = k\hat{\delta}\mathbf{i}/\hbar, \quad \omega = k^2\delta^2/2m\hbar = \boldsymbol{\kappa}\cdot\boldsymbol{\kappa}\hbar/2m.$$

The phase velocity of this wave is $\omega/|\boldsymbol{\kappa}| = k\delta/2m$ i.e. one half the velocity imposed on the wave function, and its formal group velocity is $d\omega/d\boldsymbol{\kappa} = k\hat{\delta}\mathbf{i}/m$ equal to that of the wave function itself.

1.2 The effect of a second impulse of opposite sign

Suppose at time $t=b$ (with $b > a$) we impose, all over the region W'_b of space now occupied by the wave function, a second impulse of opposite sign to the one applied at time $t=a$. Then we have over region W'_b from time $t=b$ to $t=b+\delta$ an external potential

$$V = kx$$

We again take the limit as $k \rightarrow \infty$ and $\delta \rightarrow 0$ while $k\delta$ remains finite.

By the same reasoning as in section 1.1 our wave function $\psi'(\mathbf{r}, t)$ (given by (1.1.9)) will at time $t = b$ change to $\psi''(\mathbf{r}, b)$ given by

$$\psi''(\mathbf{r}, b) = \psi'(\mathbf{r}, b)e^{-ikx\delta/\hbar} \quad (1.2.1)$$

(cf. (1.1.4)). And for $t > b$ it will be given by

$$\psi''(\mathbf{r}, t) = e^{i(-k\delta\hat{\mathbf{i}} \cdot \mathbf{r} - k^2\delta^2(t-b)/2m)/\hbar} \psi'(\mathbf{r} + k\delta\hat{\mathbf{i}}(t-b)/m, t). \quad (1.2.2)$$

(cf. (1.1.9)). Here, by (1.1.9)

$$\psi'(\mathbf{r} + k\delta\hat{\mathbf{i}}(t-b)/m, t) = e^{i[k\delta\hat{\mathbf{i}} \cdot \mathbf{r} + \frac{k^2\delta^2}{2m}(2(t-b)-(t-a))]/\hbar} \psi(\mathbf{r} - k\delta\hat{\mathbf{i}}(b-a)/m, t) \quad (1.2.3)$$

so (1.2.2) becomes

$$\psi''(\mathbf{r}, t) = e^{-ik^2\delta^2(b-a)/2m\hbar} \psi(\mathbf{r} - k\delta\hat{\mathbf{i}}(b-a)/m, t). \quad (1.2.4)$$

The effect of a second impulse of opposite sign to the first is thus to remove the bodily motion of the wave function and remove the time and position dependence of the multiplying phase factor but to leave the wave function displaced by a distance

$$D = k\delta(b-a)/m \quad (1.2.5)$$

in the x direction. Apart from the constant phase factor $e^{-ik^2\delta^2(b-a)/2m\hbar}$ and the displacement, the wave function is (for $t > b$) the same as it would have been had no impulses been applied.

1.3 Effect of a third impulse equal to the second

If at time $t = c$ we apply another impulse equal to the second (i.e. equal to $-k\delta$) we will change our wave function $\psi''(\mathbf{r}, t)$ abruptly at time $t = c$ so that (cf. (1.2.2)) for $t > c$ it will be given by

$$\psi'''(\mathbf{r}, t) = e^{i(-k\delta\hat{\mathbf{i}} \cdot \mathbf{r} - k^2\delta^2(t-c)/2m)/\hbar} \psi''(\mathbf{r} + k\delta\hat{\mathbf{i}}(t-c)/m, t). \quad (1.3.1)$$

or substituting for ψ'' using (1.2.4)

$$\psi'''(\mathbf{r}, t) = e^{i[-k\delta\hat{\mathbf{i}} \cdot \mathbf{r} - k^2\delta^2(t-c+b-a)/2m]/\hbar} \psi(\mathbf{r} + k\delta\hat{\mathbf{i}}(t-c+b-a)/m, t). \quad (1.3.2)$$

The wave function is now set in motion with velocity $-k\delta\hat{\mathbf{i}}/m$ equal and opposite to the velocity given to it by the first impulse (section 1.1). It is also multiplied by a phase factor representing a constant phase and a wave of unit amplitude with a phase velocity equal again to one half the velocity of the wave function itself.

1.4 Effect of a fourth impulse equal to the first applied

If at time $t = d$ we apply a final impulse equal to the very first applied (i.e. equal to $k\delta$) we will change our wave function $\psi'''(\mathbf{r}, t)$ abruptly at time $t = d$ so that for $t > d$ it will be given by

$$\psi^{iv}(\mathbf{r}, t) = e^{i(k\delta\hat{\mathbf{i}}\cdot\mathbf{r} - k^2\delta^2(t-d)/2m)/\hbar} \psi'''(\mathbf{r} - k\delta\hat{\mathbf{i}}(t-d)/m, t)$$

(cf. 1.1.9) or substituting for ψ''' using (1.3.2) we find that

$$\psi^{iv}(\mathbf{r}, t) = e^{i[-\frac{k^2\delta^2}{2m}(d-c+b-a)/2m]/\hbar} \psi(\mathbf{r} + k\delta\hat{\mathbf{i}}(d-c-(b-a))/m, t). \quad (1.4.1)$$

The bodily motion of the wave function is again removed but the wave function is displaced from its position at time $t = a$ by a distance

$$k\delta(d-c-(b-a))/m \quad (1.4.2)$$

in the x direction. It is also multiplied by the constant phase factor

$$e^{-i\frac{k^2\delta^2}{2m\hbar}(d-c+b-a)}. \quad (1.4.3)$$

otherwise it continues to evolve (for $t > d$) as if no impulses had been applied.

1.5 Possibility of returning the wave function to the location it had at time $t = a$

If we choose to make the time intervals between the first and second and between the third and fourth impulses equal, i.e. if we make

$$b-a = d-c \quad (1.5.1)$$

the displacement (1.4.2) is zero and the net bodily displacement of the wave function is zero. It thus evolves (for $t > d$) just as it would have done had no impulses been applied at all. The only difference is that its absolute phase is changed because of the phase factor (1.4.3).

1.6 The possibility of *instantly* displacing and returning a wave function to its original position

For simplicity let us assume the times of the second and third impulses coincide, i.e. that

$$c = b \quad (1.6.1)$$

(This is equivalent to replacing the second and third impulses by one impulse twice as strong, i.e. by an impulse of magnitude $-2kd$.) Under condition (1.5.1) our wave function is now (by (1.4.1))

$$\psi^{iv}(\mathbf{r}, t) = e^{-i\frac{k^2\delta^2}{2m\hbar}(d-a)} \psi(\mathbf{r}, t) \quad (1.6.2)$$

valid for $t > d$. Here, at time $t = d$, $\psi(\mathbf{r}, t)$ differs from its form $\psi(\mathbf{r}, a)$ at the time of the first impulse because of the natural evolution of the wave function between times a and d .

But there is nothing stopping us making time $d - a$ small compared with the characteristic time τ of variation of the undisturbed wave function $\psi(\mathbf{r}, t)$. By the free particle Schrödinger equation ((1.1.2) with $k = 0$)

$$\tau \approx \frac{2m\Delta^2}{\hbar} \quad (1.6.3)$$

where Δ is the characteristic distance of spatial variation of $\psi(\mathbf{r}, a)$. So henceforth we assume

$$d - a \ll \frac{2m\Delta^2}{\hbar}. \quad (1.6.4)$$

This does not necessarily mean that the bodily displacement D (in (1.2.5)) produced by the impulses is small. In fact it can if we like be made larger than Δ and larger than the characteristic spatial dimension Δ_{W_a} of the region W_a occupied by $\psi(\mathbf{r}, a)$. * With application to the measurement of a particle's spin component[†] in mind, we suppose this to be the case, and (since $d - a = 2(b - a)$) a necessary condition for it is (by (1.2.5)) that

$$\frac{k\delta(d - a)}{2m} > \Delta \quad (1.6.5)$$

* Clearly Δ must be less than or of the order of Δ_{W_a} and we assume here that Δ and Δ_{W_a} are of the same order.

† See section 3.1.

Now (1.6.4) and (1.6.5) together are equivalent to

$$\frac{k\delta}{\hbar} \Delta < \frac{k^2\delta^2(d-a)}{2m\hbar} \ll \frac{k^2\delta^2}{\hbar^2} \Delta^2 \quad (1.6.6)$$

which implies

$$\frac{k\delta}{\hbar} \Delta \gg 1. \quad (1.6.7)$$

The magnitude of $k^2\delta^2(d-a)/2m\hbar$ is, by (1.6.6) and (1.6.7), large compared to 1. Therefore by choice of $k\delta$ the constant phase in (1.6.2) can certainly be set (modulo 2π) to any phase from 0 to 2π . So under condition (1.6.6) the wave function $\psi(\mathbf{r},t)$ can be changed suddenly at time $t=a$ to the same function multiplied by a constant phase factor $e^{i\alpha}$ of our choosing. Formally we put

$$-\frac{k^2\delta^2(d-a)}{2m\hbar} = \alpha + 2\pi n \quad (1.6.8)$$

where α is the required constant phase in the range 0 to 2π and n is an integer, and all conditions are satisfied when we let $n \rightarrow -\infty$, $k\delta \rightarrow \infty$ and $d-a \rightarrow 0$ while $D = k\delta(d-a)/2m$ stays constant and larger than Δ_{w_a} and in fact as large as we may wish.

When using this method of instantly displacing and returning, and instantly changing the absolute phase of a wave function, we are not changing our knowledge regarding the dynamical properties of the particle and we can say that, for $t > a_+$ (i.e. just after the change in phase), our knowledge of these properties is just the same as it would have been had we not applied our impulses at all.

1.7 The possibility of returning the *particle* to its original position

In section 1.6, although the impulses are applied at time $t=a$ and the wave function is bodily displaced and returned in a vanishingly small time, this action does not essentially change our probability distribution over particle position. The wave function at time $t=a_+$ is essentially the same as it was at time $t=a_-$. And this is true whatever the initial wave function $\psi(\mathbf{r},a_-)$. Our pure knowledge concerning the dynamical properties of the particle is not changed by the action of the impulses. So our knowledge that the impulses act at time $t=a$ is redundant; it does not constitute new knowledge of the dynamical properties of the motion for $t > a_+$, and has the effect at most of introducing a known constant phase factor to the wave function.

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Now consider a series of wave functions $\psi(\mathbf{r}, t)$ for which $\psi(\mathbf{r}, a_-)$ tends to the wave function $\delta(\mathbf{r} - \mathbf{r}_1)$ which of course represents knowledge that the particle is at \mathbf{r}_1 at time $t = a_-$. Each wave function in this series will be essentially the same at $t = a_+$ as it was at $t = a_-$. And formally the limiting form $\delta(\mathbf{r} - \mathbf{r}_1)$ at $t = a_-$ will give $\delta(\mathbf{r} - \mathbf{r}_1)$ times a known constant phase factor at $t = a_+$. Hence, the proposition ‘particle is at \mathbf{r}_1 at time $t = a_-$ ’ together with our general knowledge of the laws of particle motion logically implies the proposition ‘particle is at \mathbf{r}_1 at time $t = a_+$ ’ with a *determinate* phase of implication. By the first law of extreme values of probability, this means the impulses (as applied in section 1.6) must return the particle to its previous position regardless of our particular knowledge of its motion, i.e. whatever the wave function $\psi(\mathbf{r}, a_-)$ might be. The impulses therefore instantly displace the particle a certain distance but also instantly return it exactly to the point it occupied just before the impulses were applied.

1.8 Generalisation to cases in which the particle is moving under the action of known natural potentials

Returning to the beginning of section 1, suppose our particle (known initially to be in region W_a) is not free but is moving under the action of natural local potentials $\bar{V}(\mathbf{r}, t)$ and $\bar{A}(\mathbf{r}, t)$. We suppose these potentials are zero outside regions $W_{\bar{V}}$ and $W_{\bar{A}}$ respectively (both regions enclosing region W_a) and we let $\Delta_{\bar{V}}$ and $\Delta_{\bar{A}}$ stand for the respective characteristic dimensions of regions $W_{\bar{V}}$ and $W_{\bar{A}}$.

The Schrödinger equation for $a < t < a + \delta$ during which the first impulse is applied is now

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + \bar{V} \psi + \frac{i\hbar}{m} \bar{A} \cdot \nabla \psi + \bar{A}^2 \psi - kx\psi. \quad (1.8.1)$$

As we are taking the limit $k \rightarrow \infty$ and $\delta \rightarrow 0$ while $k\delta$ remains finite it is still the case that $-kx\psi$ dominates on the RHS of (1.8.1) leading again to the expression (1.1.4) for the sudden change produced by the impulse on the wave function at time $t = a$. So again, as in (1.1.4)

$$\psi'(\mathbf{r}, a) = \psi(\mathbf{r}, a) e^{ikx\delta/\hbar} \quad (1.8.2)$$

and again (as in (1.1.7))

$$a'(\mathbf{p}, a) = a(\mathbf{p} - k\delta \hat{\mathbf{i}}, a). \quad (1.8.3)$$

But for $t > a$ we cannot generally apply the free particle Schrödinger equation. We can of course set $k = 0$ on the RHS of (1.8.1) for $t > a$, and if we substitute $\psi'(\mathbf{r}, a)$

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(of (1.8.2)) for ψ on the RHS of (1.8.1) we see that if $k\delta$ is finite but large, the dominant term on the RHS is

$$-\frac{\hbar^2}{2m}\nabla^2\psi' \approx \frac{(k\delta)^2}{2m}\psi.$$

The runner-up term is

$$\frac{i\hbar}{m}\bar{A}\cdot\nabla\psi' \approx \bar{A}\frac{k\delta}{m}\psi.$$

Since the wave function is expected to move bodily at the high velocity $k\delta/m$ for $t > a$ it will spend a time no longer than

$$\frac{\Delta_{\bar{A}}}{k\delta/m} \approx \frac{m\Delta_{\bar{A}}}{k\delta}$$

in the $\bar{A}(\mathbf{r},t)$ field, and during this time that field is expected to change ψ by an amount $\Delta\psi$ given (from (1.8.1)) by

$$-\frac{\hbar}{i}\Delta\psi \approx \frac{i\hbar}{m}\bar{A}\cdot\nabla\psi' \frac{m\Delta_{\bar{A}}}{k\delta} \approx \bar{A}\frac{k\delta}{m}\psi \frac{m\Delta_{\bar{A}}}{k\delta} \approx \bar{A}\psi\Delta_{\bar{A}}.$$

This is a fractional change of order $\bar{A}\Delta_{\bar{A}}/\hbar$ which does not become small as $k\delta$ is made larger and larger. On the other hand the terms $\bar{V}\psi$ and $\bar{A}^2\psi$ in (1.8.1) are not expected to be significant when $k\delta$ is large. The fractional changes these produce being

$$\frac{\Delta\psi}{\psi} \approx \frac{\bar{V}}{\hbar} \frac{m\Delta_{\bar{V}}}{k\delta}, \quad \frac{\Delta\psi}{\psi} \approx \frac{\bar{A}^2}{\hbar} \frac{m\Delta_{\bar{A}}}{k\delta} \quad (1.8.4)$$

which both become small when $k\delta$ is large.

In order for all the analysis in sections 1.1 to 1.7 to remain true when natural potentials are present it is therefore necessary for us to add a vector potential of our own equal and opposite to $\bar{A}(\mathbf{r},t)$ for $t > a$ or rather for the time period $a < t < d$ during which our impulses are applied. We will also need to ensure that $k\delta$ is large enough for the effect of the scalar potential to be negligible, i.e. we will have to insist (by (1.8.4)) that

$$\frac{\bar{V}m\Delta_{\bar{V}}}{\hbar k\delta} \ll 1 \quad (1.8.5)$$

for $a < t < d$. That done, equation (1.1.9) for the evolution of $\psi'(\mathbf{r}, t)$ for $t > a$ will hold well enough and so will the analysis of the effects of the second, third and fourth impulses up to and including the expression (1.4.1) for the wave function after application of the fourth impulse, and the possibility (when $d - c = b - a$) discussed in section 1.5 of returning the wave function to the position it occupied at time $t = a_-$ still applies. In section 1.6 we made the assumption that $c = b$ and that the inequalities (1.6.4) and (1.6.7) hold, or formally that (in (1.6.8)) $d - a \rightarrow 0$, $n \rightarrow \infty$ and $k\delta \rightarrow \infty$ while the displacement $D = k\delta(d - a)/2m$ produced by the impulses stays finite and larger than the width Δ_{W_a} of the region W_a occupied by the wave function at time $t = a$ and, we can now say, larger than the width $\Delta_{\bar{V}}$ of the region covered by \bar{V} . These assumptions are quite in keeping with (1.8.5) whose adoption therefore poses no problem with regard to the validity of the conclusions drawn in section 1.6 or in section 1.7. And at time $t = a_+$ after all four impulses have been applied the particle will still be returned to the position it occupied at time $t = a_-$ just before the impulses were applied. At time $t = a_+$ we should of course remove the vector potential used to cancel out the natural vector potential $\bar{A}(\mathbf{r}, t)$ so for $t > a$ the wave function $\psi(\mathbf{r}, t)$ may (apart from a possible change in absolute phase) continue as if no pulses had been applied.

We now pass to the modelling of measuring processes.

2. Measurement of a particle's position

2.1 Harmless conditioning with regard to particle position

Suppose we have a pure state of knowledge regarding the orbital motion of a particle moving perhaps under the action of known local potentials $\bar{V}(\mathbf{r}, t)$ and $\bar{A}(\mathbf{r}, t)$. Let $\psi(\mathbf{r}, t)$ be the wave function over position representing this pure knowledge. We suppose $\psi(\mathbf{r}, t)$ tends to zero fast enough as $|\mathbf{r}| \rightarrow \infty$ so that we may effectively claim we know the particle lies within a finite region W of fixed space for a certain period of time. Then at any specified time $t = a$ during that period we have claimed (see section 3.6 of Chapter I) that we may, by chance, be able to establish that the particle is in fact in a prescribed smaller region W_1 (within W). And we can do this harmlessly with regard to particle position at the time in question. We now model a method for doing this.

Method:

Everywhere in W we temporarily apply a vector potential $A(\mathbf{r}, t)$ equal and opposite to $\bar{A}(\mathbf{r}, t)$ so as to reduce the net vector potential to zero, and from time $t = a$ to $t = a + \delta$ we apply to the region $W - W_1$ (which we call W_2) a scalar potential with a large constant gradient k and take the limit as $k \rightarrow \infty$ and $\delta \rightarrow 0$ while $k\delta$ remains finite (and large).

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Then if no particle in classical motion is observed far away shortly after time $t = a$, we remove our applied vector potential $\mathbf{A}(\mathbf{r}, t)$ and establish, harmlessly with regard to particle position at the time in question, that the particle is in W_1 at time $t = a$.

Modelling of the method:

During the small time interval $a < t < a + \delta$ let the applied potential be

$$V = -kx \quad (2.1.1)$$

everywhere in the region W_2 and zero everywhere else* (see Figure 2.1.1). In (2.1.1) k is a real positive constant so the potential gradient is in the negative x direction of the fixed coordinates. We take the limit $k \rightarrow \infty$ and $\delta \rightarrow 0$ while the 'impulse' $k\delta$ in the positive x direction remains finite and large. The impulse field is illustrated by the arrows in Figure 2.1.1.

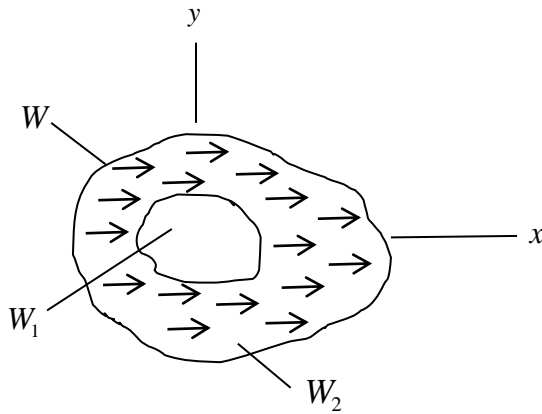


Figure 2.1.1

For $t > a$ let the wave function be split into two parts:

$$\psi(\mathbf{r}, t) = \psi_1(\mathbf{r}, t) + \psi_2(\mathbf{r}, t) \quad (2.1.2)$$

where $\psi_1(\mathbf{r}, a)$ equals $\psi(\mathbf{r}, a)$ in region W_1 but is zero in region W_2 , and $\psi_2(\mathbf{r}, a)$ equals $\psi(\mathbf{r}, a)$ in region W_2 but is zero in region W_1 . For $t > a$ let $\psi_1(\mathbf{r}, t)$ evolve according to the Schrödinger equation under the action of both the natural potentials and the applied potentials and let $\psi_2(\mathbf{r}, t)$ evolve according to the Schrödinger equation under the action

* In the case the particle carries a charge, V could be an electric potential created by sources in the boundary between W_1 and W_2 and in the boundary between W_2 and the surrounding space (cf. first footnote in section 1.1).

of both the natural potentials and the applied potentials. The sum $\psi_1(\mathbf{r},t) + \psi_2(\mathbf{r},t)$ will then satisfy the Schrödinger equation with all potentials present.

In the evolution of $\psi_1(\mathbf{r},t)$, for $a < t < a + \delta$, there will be vanishingly small penetration of $\psi_1(\mathbf{r},t)$ into W_2^* so $\psi_1(\mathbf{r},t)$ is hardly changed. But in W_2 the applied potential dominates over all other terms on the RHS of the Schrödinger equation. So we have, for $\psi_2(\mathbf{r},t)$:

$$-\frac{\hbar}{i} \frac{\partial \psi_2}{\partial t} = -kx\psi_2 \quad (2.1.3)$$

with solution

$$\psi_2(\mathbf{r},t) = \psi_2(\mathbf{r},a)e^{ikx(t-a)/\hbar}.$$

Since $\delta \rightarrow 0$ we can say the impulse $k\delta$ of the applied potential changes $\psi_2(\mathbf{r},a)$ instantly to

$$\psi'_2(\mathbf{r},a) = \psi_2(\mathbf{r},a)e^{ikx\delta/\hbar} \quad (2.1.4)$$

within region W_2 and leaves it zero inside region W_1 . The wave function $\psi_2(\mathbf{r},a)$ has become a wave packet $\psi'_2(\mathbf{r},a)$ containing many de Broglie wavelengths and the work carried out in section 1.1 (and its generalisation in section 1.8) shows that because we are taking $k\delta$ to be large the wave function $\psi'_2(\mathbf{r},t)$ for $t > a$ is given by

$$\psi'_2(\mathbf{r},t) = e^{i(k\delta\hat{\mathbf{i}}\cdot\mathbf{r} - k^2\delta^2(t-a)/2m)/\hbar} \psi_2(\mathbf{r} - k\delta\hat{\mathbf{i}}(t-a)/m, t). \quad (2.1.5)$$

where on the RHS the function $\psi_2(\mathbf{r},t)$ denotes the (comparatively slowly changing) wave function evolving from its form $\psi_2(\mathbf{r},a)$ at $t = a$ assuming zero net vector potential present and no impulse applied. This confirms that $\psi'_2(\mathbf{r},t)$ remains for all time a wave packet containing many de Broglie wavelengths, and one moving with a high velocity \mathbf{v} given by

$$\mathbf{v} = \frac{k\delta}{m} \hat{\mathbf{i}}. \quad (2.1.6)$$

At very short times after the action of the impulse our total wave function is

$$\psi'(\mathbf{r},t) = \psi'_1(\mathbf{r},t) + \psi'_2(\mathbf{r},t) \quad (2.1.7)$$

* See Appendix G for a quantitative study of the rate of penetration of a wave function into a region where it is initially zero.

where $\psi'_1(\mathbf{r}, t)$ is hardly different from its initial form $\psi_1(\mathbf{r}, a)$ (which is confined to region W_1) and $\psi'_2(\mathbf{r}, t)$ is a fast moving (unnormalised) quasi-classical wave packet* already far from region W_1 and therefore not overlapping $\psi'_1(\mathbf{r}, t)$. By the *law of motion under a part quasi-classical wave function* (see section 1.4 of Chapter XII) the particle may (to classical accuracy) be moving classically as it would under the quasi-classical wave function $\psi'_2(\mathbf{r}, t)$ alone. And the modulus squared of the probability for this is

$$\int |\psi'_2(\mathbf{r}, t)|^2 d^3\mathbf{r},$$

where the integral is over all space. Such a motion would be directly observable and in the event that, by chance, no such motion is observed we learn that the particle must be in region W_1 . Furthermore, by the first law of potential action (section 3.2 of Chapter III), its motion could not have been affected by our applied potential gradient because the particle (not moving infinitely fast) could not (during the action of the applied potential) have moved into the region W_2 where the potential was applied. Therefore, in the absence of a particle observed in classical motion very shortly after the applied potential impulse, we have acquired the knowledge (that the particle occupies region W_1 at time $t = a$) *harmlessly* with regard to the particle's position at time $t = a$. Our initial wave function $\psi(\mathbf{r}, a)$ collapses (effectively instantaneously[†]) to $\psi_1(\mathbf{r}, a)$ (as defined by (2.1.2)) multiplied by a positive normalisation factor and an indeterminate constant phase factor (as follows from the general result (4.2) of Chapter II). Our applied vector potential $\mathbf{A}(\mathbf{r}, t)$ (used to cancel out the natural vector potential $\bar{\mathbf{A}}(\mathbf{r}, t)$) may now be removed.

We thus see how the proposed method for performing harmless conditioning with regard to particle position operates in a way wholly consistent with the laws of quantum mechanics.

2.2 Exact measurement of particle position

A particular case of harmless conditioning with regard to particle position is of course the case in which the volume W_1 in section 2.1 is taken arbitrarily small so it becomes (in the limit) an infinitesimal volume element at a position \mathbf{r}_1 . We thus see how, when starting

* Clearly, the expression (2.1.5) for $\psi'_2(\mathbf{r}, t)$ for $t > a$ has the form of the simplest kind of quasi-classical wave function ((1.2.1) of Chapter XII) since its phase (like $S(\mathbf{r}, a)/\hbar$ in (1.2.1) of Chapter XII) is $\gg 1$ and changes very rapidly with \mathbf{r} and t . The modulus squared of $\psi'_2(\mathbf{r}, t)$ is the classical probability distribution over particle position when its motion (under knowledge $\psi'_2(\mathbf{r}, t)$) is viewed to classical accuracy.

[†] This requires of course that $k\delta$ is large enough for us to be able to null-detect a particle in classical motion in a time short compared to the characteristic time in which $\psi_1(\mathbf{r}, t)$ varies significantly.

out with pure knowledge of a particle's motion, we might find (by chance) the position actually occupied by the particle at a given time. This confirms the possibility in principle of measuring the (primary) basic property of particle position to quantum mechanical accuracy at any time during single particle motion under a pure state of knowledge. The effect of such a measurement is to instantly collapse our wave function $\psi(\mathbf{r}, a)$ to $\delta(\mathbf{r} - \mathbf{r}_1)$ times a generally indeterminate phase factor (as in the special case (4.3) of Chapter II).

2.3 Generation of the impulsive potentials

In preparation for the arguments in section 2.4 and out of general interest we consider how the potential in (2.1.1) might be generated in the case it is an electric potential and the particle undergoing measurement carries a unit charge.

Since nature provides us only with charged particles, not with continuously distributed charge (either over volumes or surfaces) we must seek to model potential generation using charged particles. These may be of any charge* and mass and taking their masses to be extremely large they can be assumed to move classically under the action of any applied (non-electromagnetic) forces we please. They can therefore move in any manner we please and are not themselves affected by the electric fields they generate or by the particles they are set up to interact with.

To create the potential (2.1.1) during the time period $a < t < a + \delta$ we assemble a swarm of N charged particles half of which have charge q and half of which have charge $-q$. We distribute the particles of +ve charge (and those of -ve charge) uniformly in regions R of space of constant thickness Δ_l over the inside of the boundary of W_1 and over the outside of the boundary of W_2 (Figure 2.3.1).

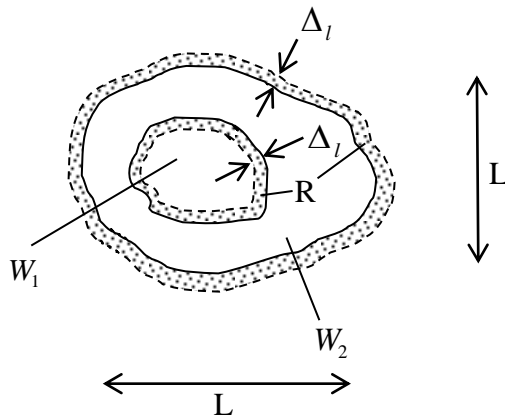


Figure 2.3.1

* Although the particles of nature may have charges that are multiples of the charge of the electron, there is nothing in quantum mechanics that dictates this must be the case. That is, in principle, quantum mechanical particles may have any charge (as well as any mass).

On taking the limits

$$q \rightarrow 0, N \rightarrow \infty, \Delta \rightarrow 0, \Delta_l = \text{const.} \quad (2.3.1)$$

where Δ is the order of magnitude of the distance between any one charge and its neighbour and taking

$$q \sim \Delta^p \quad (p > 2), \quad N \sim \frac{1}{\Delta^3} \quad (2.3.2)$$

where \sim is used to denote the ‘same limiting order as’, we ensure the electric potential and electric field is effectively zero everywhere. This is because the net charge density in R is always zero so no overall field is produced, and the average electric field at a point P in R is of the order

$$\frac{1}{\Delta^3} \int_0^\Delta \frac{q}{r^2} r^2 dr \approx \frac{1}{\Delta^3} q \Delta \sim \Delta^{p-2}$$

where r is the distance from P to the nearest source particle, and $\Delta^{p-2} \rightarrow 0$. * Put another way, if an electric field of strength E (or greater) is considered significant (with regard to its effect on the particle undergoing measurement) then such a field strength is present only within a distance d from a source charge where

$$\frac{q}{d^2} \approx E$$

i.e. only within a distance $d \approx (q/E)^{1/2}$ of a source charge. But the relative volume of space to which this applies is of order

$$\frac{d^3}{\Delta^3} \approx \frac{(q/E)^{3/2}}{\Delta^3} \sim E^{-\frac{3}{2}} \Delta^{\frac{3}{2}p-3}$$

which tends to zero in the limit $\Delta \rightarrow 0$ for any assigned value of E however small.†

The charges assembled in this way are supposed to be present and so assembled up to time $t = a$ and from time $t = a + \delta$ onward. During these times they have no effect on the particle undergoing measurement. But during time $a < t < a + \delta$ we suppose the

* The average electric potential is likewise of order Δ^{p-1} and also tends to zero in the limit.

† Similarly, if a potential ϕ (or greater) is considered significant, then with $q/d \approx \phi$, $d^3/\Delta^3 \sim \phi^{-3} \Delta^{3p-3}$ tends to zero for any ϕ .

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assembled charges are moved suddenly (at time $t = a$) to new positions and returned (at time $t = a + \delta$) to their original positions.*

During times $a < t < a + \delta$ we suppose the same charges lie within a region R' like R (in Figure 2.3.1) but of thickness Δ'_l ($\ll \Delta_l$). The charges of +ve sign are no longer uniformly distributed (in R'). A measure of charge separation has occurred, both within the thickness of layer R' and over it, so as to produce a net surface charge density and a net (normally directed) dipole density as needed to generate the potential (2.1.1). There will now be a normally directed electric field E' inside R' creating a potential jump of order $E'\Delta'_l$ across layer R' (varying of course from place to place over the layer). Since the required potential gradient in W_2 is k we must have

$$E'\Delta'_l \approx kL \quad (2.3.3)$$

where L is the characteristic length of W . This makes

$$E' \gg k$$

indicating that the charge separation across the thickness Δ'_l of the layer R' is almost complete over most of R' . Because of this, a simple application of Gauss's theorem gives

$$E' \approx \frac{Nq}{L^2} \quad (2.3.4)$$

Combining (2.3.3) and (2.3.4) we get

$$\frac{Nq}{L^2} \Delta'_l \approx kL \quad (2.3.5)$$

giving us the order of magnitude of Nq required to generate any needed electric field strength k in region W_2 .

Applying the necessary limiting process ((2.3.1) and (2.3.2)) we see that

$$Nq \sim \frac{1}{\Delta^3} \Delta^p \sim \Delta^{p-3}$$

and by further proposing that

$$\Delta'_l \approx \Delta^s \quad (s > 0) \quad (2.3.6)$$

* These sudden motions cause no currents with associated magnetic potentials in our (non-relativistic) electrodynamic theory (in Appendix C) but they might do so (and cause problems for us) in measurement theory in relativistic quantum theory.

we have

$$k \approx \frac{Nq}{L^3} \Delta'_l \sim \Delta^{p-3+s} \quad (2.3.7)$$

and we can arrange for $k \rightarrow \infty$ (as required) by insisting that $p-3+s < 0$. Then of course, since $k\delta$ remains constant we have

$$\delta \sim \Delta^{-p+3-s} \quad (2.3.8)$$

tending to zero in the limit.

Because the number of source particles at any step in the limiting process is the same for $a < t < a + \delta$ as for $t < a$ and $t > a + \delta$, we have

$$N\Delta^3 \approx \Delta_l L^2 \quad \text{and} \quad N\Delta'^3 \approx \Delta'_l L^2 \quad (2.3.9)$$

where Δ' is the order of magnitude of the distance between any one source particle and its nearest neighbour again assuming uniform order of magnitude of Δ' (everywhere in R'). From (2.3.9) we obtain

$$\Delta'^3 \approx \frac{\Delta'_l}{\Delta_l} \Delta^3 \sim \Delta^{s+3}$$

or

$$\Delta' \sim \Delta^{\frac{s+3}{3}} \quad (2.3.10)$$

We note finally the absence of any direct effect of any source particle on the particle undergoing measurement. For during time $a < t < a + \delta$ the average electric field at a point P near any one source charge is

$$\frac{1}{\Delta'^3} \int_0^{\Delta'} \frac{q}{r^2} r^2 dr \approx \frac{1}{\Delta'^3} q\Delta' \sim \Delta^{p-\frac{2s}{3}-2}$$

which tends to zero* provided

* Likewise the average potential $\approx q/\Delta' \sim \Delta^{p-\frac{s}{3}-1}$ tends to zero under (2.3.11). Or, if E is considered significant then with $q/d^2 \approx E$, $d^3/\Delta'^3 \sim \Delta^{\frac{3}{2}p-s-3} \rightarrow 0$; and if ϕ is considered significant then with $q/d \approx \phi$, $d^3/\Delta'^3 \sim \Delta^{3p-s-3} \rightarrow 0$.

$$p - \frac{2s}{3} - 2 > 0. \quad (2.3.11)$$

Taken all together, the requirements for p and s are

$$\left. \begin{array}{l} p > 2 \\ s > 0 \\ p - 3 + s < 0 \\ p - \frac{2s}{3} - 2 > 0 \end{array} \right\} \quad (2.3.12)$$

These can be satisfied simultaneously by taking the Cartesian coordinates (p, s) of a point in the ps plane to lie in the triangle $((2,0), (3,0), (\frac{12}{5}, \frac{3}{5}))$.

2.4 The possible effect of the measurement of a particle's position on its momentum

We claimed in section 2.1 that the process of harmless conditioning with respect to particle position, i.e. the successful instant location of particle position somewhere within region W_1 , does not affect the particle's motion because the particle could not have moved (in the vanishingly short time δ) from region W_1 to region W_2 and therefore could not have experienced the applied potential.

This would suggest that the particle's momentum as well as its position is always left unaffected by the measurement. However, at least in the case the particle carries charge (we take to be of unit magnitude for simplicity) and the potential (2.1.1) is an electric potential, there is reason to think the particle's momentum could be affected. This is because of the presence of a large electric field E' inside the boundary between W_1 and W_2 . In fact $E' \rightarrow \infty$ in the limiting process in section 2.3 and does so faster than k does and in such a way that $E'\Delta'_l$ and kL stay the same in order of magnitude even as $\Delta'_l \rightarrow 0$ (see (2.3.3)). And this leads us to expect the momentum of the particle might be affected.

To be more specific, consider the case our position measurement is specialised to a measurement of the x coordinate of the particle. That is, suppose W_1 is a region

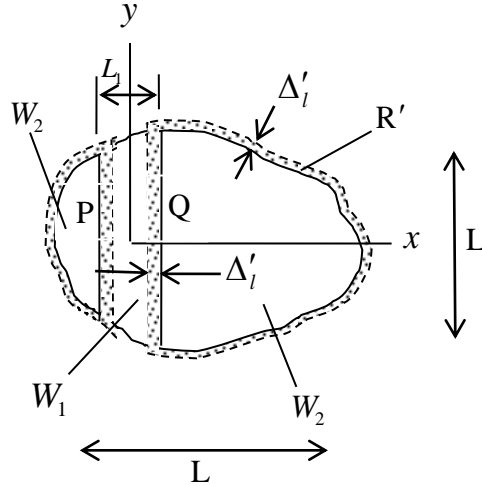


Figure 2.4.1

bounded within W by planes P and Q perpendicular to the x axis distance L_1 apart (Figure 2.4.1). Take the origin of coordinates half way between P and Q . To realise the potential (2.1.1) over W_2 the order of magnitude of $E'\Delta'_l$ in the parts of R' over planes P and Q must be equal to the jump in potential (in W) from zero at distance Δ'_l to the right of P and distance Δ'_l to the left of Q to $\pm kL_1/2$ just to the left of P or just to the right of Q . So in those parts of R' we have in place of (2.3.3)

$$E'\Delta'_l \approx kL_1. \quad (2.4.1)$$

In order for the particle to remain either in W_1 or in W_2 during the measurement it is necessary that under its natural drifting velocity v_x it should not have time to travel distance Δ'_l . That is, the time δ must be less than Δ'_l/v_x . So δ must tend to zero faster than Δ'_l , i.e. by (2.3.8) and (2.3.6)

$$-p + 3 - s > s \quad (2.4.2)$$

which is quite possible (under (2.3.12)) and we assume it is the case.*

Immediately after successful harmless conditioning leading to knowledge that the particle's x coordinate lies between $x = -\frac{1}{2}L_1$ and $x = \frac{1}{2}L_1$ our (un-normalised) wave function is ψ_1 (as defined in (2.1.2)) and our relative degree of belief the particle occupied (during action of the applied potential) a point in the part of R' over plane P or

* If instead of claiming momentum is an internal property of a particle we were to claim it was a property associated with its drifting velocity through space, the field E' would (if the particle was in region R') produce a large increase in this drifting velocity and it would not be possible to ensure the particle stayed in region W_1 if it started there during measurement. That is, harmless conditioning with respect to particle position would be impossible.

Q is of the order $|\psi_1|^2 \Delta'_1 L^2$ and our expected value $\overline{\Delta p_x}$ for the x component of momentum imparted to it by E' in the time δ is

$$\overline{\Delta p_x} \approx \frac{E'\delta|\psi_1|^2 \Delta'_1 L^2 + 0 \cdot |\psi_1|^2 L_1 L^2}{|\psi_1|^2 L_1 L^2} \approx \frac{E'\delta \Delta'_1}{L_1} \approx k\delta \quad (2.4.3)$$

the last step following from (2.4.1). The time t_M of the measurement must have been long enough for the wave function ψ_2 to have been moved well clear of the region W . Since the velocity imparted to ψ_2 was $k\delta/m$ we need

$$\frac{k\delta}{m} t_M \gg L.$$

But, for harmless conditioning, the same measurement must also have been performed in a time small compared to the time $\approx mL_1^2/\hbar$ of natural evolution of ψ_1 , i.e.

$$t_M \ll \frac{mL_1^2}{\hbar}.$$

Hence

$$k\delta \gg \frac{Lm}{t_M} \gg Lm \frac{\hbar}{mL_1^2} \approx \hbar \frac{L}{L_1^2}.$$

If we write L_1 as $\overline{\Delta x}$ to represent our uncertainty in the x coordinate of the particle after the measurement, the above result (with (2.4.3)) gives

$$\overline{\Delta p_x} \overline{\Delta x} \approx k\delta \cdot L_1 \gg \hbar \frac{L}{L_1}. \quad (2.4.4)$$

And because $L_1 \leq L$ and our uncertainty in p_x is at least equal to $\overline{\Delta p_x}$, result (2.4.4) conforms to the uncertainty principle relation $\overline{\delta p_x} \overline{\delta x} \geq \hbar/2$ between standard deviations $\overline{\delta x}$ and $\overline{\delta p_x}$ (as derived for example in section 11.8 of [10]). We note that (2.4.4) represents a degree of uncertainty in position and momentum much greater than is actually dictated by the uncertainty principle itself. This has to do with our requirement for harmless conditioning with regard to particle position.*

* In perfect harmless conditioning ψ_1 generally falls abruptly to zero on crossing planes P and Q out of region W_1 into region W_2 , and the standard deviation $\overline{\delta p_x}$ in the momentum representation of state ψ_1 is

The relationship between the uncertainty principle and the degree of disturbance inflicted by measurements is not simple. One has to distinguish between the alteration in uncertainty due to a change in our knowledge (resulting from a measurement) and the physical disturbance produced by the measurement. If for example the wave functions ψ_1 and ψ_2 in (2.1.2) were confined to regions well within W_1 and W_2 , then ψ_1 would be zero in R' and instead of (2.4.3) we would have $\overline{\Delta p_x} = 0$, i.e. successful harmless conditioning would leave the particle's momentum (as well as its position) unchanged. The alteration in the probability distribution over momentum (generally associated with the change from ψ to ψ_1) is then a result of the change in our knowledge alone. So according to our interpretation of quantum mechanics acquisition of more exact (pure) knowledge of one of a pair of properties (knowledge of which is limited by the uncertainty principle) does not always affect the other property physically. And our knowledge of that other property may become less precise *or* more precise.*

3. Measurement of a particle's spin component as well as its position

3.1 Harmless conditioning with respect to a particle's spin component

Suppose we have a pure state of knowledge regarding the orbital *and* spinning motion of a particle of spin s moving perhaps under the action of known natural (finite) potentials (including a finite magnetic field of any known space and time variation). Let our pure knowledge be represented by the wave function $\psi_\sigma(\mathbf{r}, t)$ over position \mathbf{r} and spin component σ relative to a fixed Cartesian coordinate system, σ of course taking values $-s, -s+1, \dots, s$. We suppose that, for all σ , $\psi_\sigma(\mathbf{r}, t)$ tends to zero rapidly enough as $|\mathbf{r}| \rightarrow \infty$ so that we may again effectively claim we know the particle lies within a finite region W of fixed space for a certain period of time.

Now $\psi_\sigma(\mathbf{r}, t)$ is a (generally inseparable) wave function in the combined sample space $S_\sigma S_r$ of the complete sample spaces S_r and S_σ of propositions regarding the orbital and spinning motions respectively relative to fixed Cartesian coordinate systems. As we have said before, a basis in S_r claiming one or other particle position coordinates at any particular time is a *primary* basis, so is a basis in S_σ claiming one or other particle spin component in the same coordinate system at any particular time, therefore the basis

accordingly infinite. This is consistent with (2.4.3) when we consider that $k\delta$ must tend to infinity for perfect harmless conditioning.

* For example, if ψ_1 and ψ_2 are wave packets each representing fairly well known (and different) particle momenta, and these packets lie (at time $t = a$) well within W_1 and W_2 respectively, then after harmless conditioning (which is harmless both with regard to particle position *and* its momentum) our knowledge of particle momentum becomes *more* precise (not less precise). Such is the situation in the particle interferometer of section 1.3 Chapter XII when we null detect (fail to detect) the particle in one arm of the interferometer –our knowledge of particle momentum is then instantly made more precise, but at a later time, when the particle has left the interferometer, our knowledge of the momentum becomes as uncertain as it was just before the null measurement.

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in $S_\sigma S_r$, claiming one or other position coordinate *and* one or other spin component at any particular time is a primary basis.

Accordingly, in sample space $S_\sigma S_r$ and with regard to our chosen fixed Cartesian coordinate system, it must be possible for us to establish by chance, at any specified time t , that the particle has in fact a particular spin component σ_1 or that its spin component is one or other of a certain set $\{\sigma_1, \dots, \sigma_n\}$ of n different spin component values. And we can do this harmlessly with regard to its spin component and its position at the time in question. This is harmless conditioning with respect to the spin component in $S_\sigma S_r$. We now model a method for doing this which (like the method proposed by Feynman et al in section 5-1 of [7]) employs a magnetic field with a large spatial gradient.

Method:

Everywhere in the region W where the particle is known to be we temporarily apply a vector potential equal and opposite to any vector potential present, and for a vanishingly short time from $t = a$ to $t = a + \delta$, we apply a magnetic field in the z direction with a gradient k in the x direction. We take the limit as $k \rightarrow \infty$ and $\delta \rightarrow 0$ while the ‘impulse’ $k\delta$ remains finite. (*Classically* this would produce an impulse on the particle proportional to its z component of spin and arising from the fact that (from $t = a$ to $t = a + \delta$) the energy of its magnetic moment in the field changes rapidly with its x coordinate implying a large force on the particle in the x direction.) At $t = b$, shortly after $t = a$, the result, for a large enough impulse $k\delta$, is a separation of the wave function $\psi_\sigma(\mathbf{r}, t)$ in space into as many separate parts as there are possible spin component values σ . During a further vanishingly small time interval from $t = b$ to $t = b + \delta$ we take away the high velocity of those separate wave packets for which $\sigma \in \{\sigma_1, \dots, \sigma_n\}$ by applying to them (and only to them) a magnetic field impulse equal and opposite to the one we first applied. And if the set $\{\sigma_1, \dots, \sigma_n\}$ excludes the case $\sigma = 0$ we apply a scalar potential gradient pulse over region W to send the particle to infinity if its spin is zero. Finally, to return the wave functions $\psi_\sigma(\mathbf{r}, t)$ for which $\sigma \in \{\sigma_1, \dots, \sigma_n\}$ to their initial forms we subject them immediately to another magnetic field impulse equal and opposite to the one we first applied to send these wave functions on their way back and after the short time interval $b - a$, when they have arrived back, we bring them to rest using a magnetic field impulse the same as the one we first applied. Provided the whole operation is completed in a vanishingly short time and provided no particle is observed in classical motion far away we can conclude that $\sigma \in \{\sigma_1, \dots, \sigma_n\}$ both at time $t = a$ (before all our fields were applied) and just after (when the natural vector potential may be restored), and we have achieved our objective of harmless conditioning with respect to the spin component.

Modelling of the method:

Take the origin of coordinates somewhere in W (see Figure 3.3.1.) and let our first

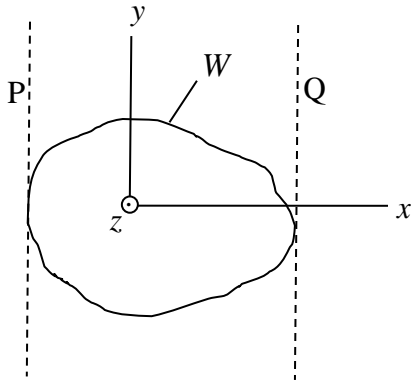


Figure 3.1.1

magnetic field \mathbf{H} be applied in the region between two planes P and Q which are parallel to the yz plane and positioned on either side of region W with \mathbf{H} given everywhere in W by

$$\mathbf{H} = kx\hat{\mathbf{k}} \quad (3.1.1)$$

where k is a constant and $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$ stand for the unit vectors in the x , y and z directions. This \mathbf{H} field must be due to an electromagnetic vector potential which in W is of the form

$$\mathbf{A}_{\text{em}} = \left(\frac{1}{2}kx^2 + \text{const.}\right)\hat{\mathbf{j}} \quad (3.1.2)$$

the curl of which gives $kx\hat{\mathbf{k}}$. * (If the particle has charge q this will add orbital terms to the Schrödinger equation associated with the particle vector potential $\mathbf{A} = q\mathbf{A}_{\text{em}}/c$.)

Since \mathbf{H} has only a z component in W the Schrödinger equation during time $t = a$ to $t = a + \delta$ is (by (6.2.6) of Chapter IX)

$$-\frac{\hbar}{i} \frac{\partial \psi_{\sigma}}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi_{\sigma} + \bar{V} \psi_{\sigma} - \frac{\sigma}{s} \mu H_z \psi_{\sigma} \quad (3.1.3)$$

* Since, by (3.1.1), $\nabla \times \mathbf{H} = -k\hat{\mathbf{j}}$ a uniform current density in the y direction must be present throughout W where the particle is situated. That this can be done without affecting the particle motion directly is argued in the part of Appendix C headed *Note on the relativistic modelling of electromagnetic field sources*. To obtain the required values of \mathbf{A}_{em} in W the current density between planes P and Q need not extend all the way to infinity in the y and z directions but can be terminated at distances far enough away from W .

where \bar{V} is the (finite) natural scalar potential (the natural vector potential and the vector potential $q\mathbf{A}_{\text{em}}/c$ (if present) are assumed to be cancelled out) and H_z is as given in (3.1.1). We thus have a separate Schrödinger equation for each spin component $\sigma = -s, -s+1, \dots, s$.*

Since we are taking the limit as $\delta \rightarrow 0$ and $k \rightarrow \infty$ while $k\delta$ remains finite, the first two terms on the RHS of (3.1.3) will have zero effect and can therefore be omitted, giving

$$-\frac{\hbar}{i} \frac{\partial \psi_\sigma}{\partial t} = -\frac{\sigma}{s} \mu k x \psi_\sigma. \quad (3.1.4)$$

Thus for $\sigma=0$ the magnetic field applied during time $t=a$ to $t=a+\delta$ leaves ψ_σ unchanged but for $\sigma \neq 0$ the wave function $\psi_\sigma(\mathbf{r}, t)$ is changed in the same way as $\psi(\mathbf{r}, t)$ is changed in section 1.1 under a net effective potential V given by

$$V = -\frac{\sigma}{s} \mu k x. \quad (3.1.5)$$

So $\psi_\sigma(\mathbf{r}, t)$ (for any value of σ) becomes (cf. (1.1.4))

$$\psi'_\sigma(\mathbf{r}, a) = \psi_\sigma(\mathbf{r}, a) e^{i \frac{\sigma}{s} \mu \frac{kx\delta}{\hbar}} \quad (3.1.6)$$

representing (when $\sigma \neq 0$) a quasi-classical wave packet of high velocity (assuming, as we do, that $k\delta$ is large).

Shortly after time $t=a$ and on account of $k\delta$ being large, the wave function $\psi'_\sigma(\mathbf{r}, t)$ is therefore the sum of several parts well separated in configuration space, i.e.

$$\psi'_\sigma(\mathbf{r}, t) = \sum_{\sigma'=-s}^s \delta_{\sigma\sigma'} \psi'_{\sigma'}(\mathbf{r}, t). \quad (3.1.7)$$

Each term $\delta_{\sigma\sigma'} \psi'_{\sigma'}(\mathbf{r}, t)$ in the sum is a (unnormalised) wave function representing knowledge of a particle moving with a distinct spin component σ' in a separate region of space. The term with $\sigma'=0$ (i.e. $\delta_{\sigma 0} \psi'_0(\mathbf{r}, t)$) represents knowledge of a particle with zero spin component unaffected by the applied impulse but still well separated in space

* If there is a natural magnetic field $\bar{\mathbf{H}}$ present we do not generally have a separate Schrödinger equation for each spin component. Instead the equations for the time derivatives of the wave functions for each spin component are linked by terms involving \bar{H}_x and \bar{H}_y (see for example the Schrödinger equation (9.1.4) of Chapter VII). However, as the applied field H_z tends to infinity, the terms involving \bar{H}_x and \bar{H}_y linking the wave functions with different spin components become negligible like the term involving \bar{V} in (3.1.3).

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from the regions occupied by the other terms. The terms with $\sigma' \neq 0$ (taken together) form a superposition of quasi-classical wave functions any one of which is for a classical particle with a definite spin component and a very high velocity proportional to its spin component. For times shortly after time $t=a$ the expression for the spatial factor $\psi'_{\sigma'}(\mathbf{r}, t)$ of any of the wave functions in the summand of (3.1.7) is

$$\psi'_{\sigma'}(\mathbf{r}, t) = e^{i[\frac{\sigma'}{s}\mu k\delta\hat{\mathbf{i}}\cdot\mathbf{r} - \frac{\sigma'^2}{s^2}\mu^2 k^2\delta^2(t-a)/2m]/\hbar} \psi_{\sigma'}(\mathbf{r} - \frac{\sigma'}{s}\mu k\delta\hat{\mathbf{i}}(t-a)/m, t) \quad (3.1.8)$$

(cf. (1.1.9)) where $\psi_{\sigma'}(\mathbf{r}, t)$ denotes the wave function $\psi_{\sigma}(\mathbf{r}, t)$ (with $\sigma = \sigma'$) evolving comparatively slowly and naturally from its original form $\psi_{\sigma}(\mathbf{r}, a)$ at $t=a$ with no net vector potential and no applied impulse.

Shortly after time $t=a$ at time $t=b$ the spatial factors $\psi'_{\sigma'}(\mathbf{r}, t)$ of wave functions $\delta_{\sigma\sigma'}\psi'_{\sigma'}(\mathbf{r}, t)$ will be well separated in the x direction and those for which $\sigma' \in \{\sigma_1, \dots, \sigma_n\}$ and $\sigma' \neq 0$ may, during time $t=b$ to $t=b+\delta$, be brought to rest by application to each of them of a magnetic field gradient impulse equal and opposite to the one first applied. The $\psi'_{\sigma'}(\mathbf{r}, b)$ (for $\sigma' \neq 0$) are thus instantly changed to

$$\psi''_{\sigma'}(\mathbf{r}, b) = e^{i[-\frac{\sigma'}{s}\mu k\delta\hat{\mathbf{i}}\cdot\mathbf{r}]/\hbar} \psi'_{\sigma'}(\mathbf{r}, b)$$

(cf. (1.2.1)), and for $t > b$ they take the form

$$\psi''_{\sigma'}(\mathbf{r}, t) = e^{i[-\frac{\sigma'}{s}\mu k\delta\hat{\mathbf{i}}\cdot\mathbf{r} - \frac{\sigma'^2}{s^2}\mu^2 k^2\delta^2(t-b)/2m]/\hbar} \psi'_{\sigma'}(\mathbf{r} + \frac{\sigma'}{s}\mu k\delta\hat{\mathbf{i}}(t-b)/m, t)$$

(cf. (1.2.2)), and substituting for $\psi'_{\sigma'}$ using (3.1.8) gives, for $t > b$,

$$\psi''_{\sigma'}(\mathbf{r}, t) = e^{-i\frac{\sigma'^2}{s^2}\mu^2 k^2\delta^2(b-a)/2m\hbar} \psi_{\sigma'}(\mathbf{r} - \frac{\sigma'}{s}\mu k\delta\hat{\mathbf{i}}(b-a)/m, t) \quad (3.1.9)$$

(cf. 1.2.4). And (3.1.9) holds also when $\sigma' = 0$, i.e. for the wave function $\psi''_0(\mathbf{r}, t)$ unaffected by our magnetic field impulses. So the velocities of $\psi''_{\sigma'}$ (for $\sigma' \neq 0$) are now stopped but they each remain displaced (in the x direction) from their original position by distances $D' = \frac{\sigma'}{s} \frac{\mu k\delta}{m} (b-a)$ which (by choice of $k\delta$) we are supposing large enough to spatially separate the functions $\psi''_{\sigma'}$ for all the various values of σ' . Since successive σ' values differ by 1 this requires

$$\frac{\mu}{s} \frac{k\delta(b-a)}{m} > \Delta_{\sigma'} \quad (3.1.10)$$

for $\sigma' = -s, -s+1, \dots, s$ where $\Delta_{\sigma'}$ is the dimension of the region of space occupied by the wave function $\psi_{\sigma'}$.

If $\{\sigma_1, \dots, \sigma_n\}$ excludes the spin component $\sigma=0$ we now apply a scalar potential field impulse over the region occupied by $\psi_0(\mathbf{r}, t)$ to send this wave function on its way to infinity. And to those wave packet functions $\psi_{\sigma'}$ for which $\sigma' \in \{\sigma_1, \dots, \sigma_n\}$ and $\sigma' \neq 0$ we immediately follow up the negative magnetic field gradient impulse by another one equal to it. This changes the functions $\psi_{\sigma'}$ (for $\sigma' \in \{\sigma_1, \dots, \sigma_n\}$ and $\sigma' \neq 0$) to functions $\psi_{\sigma'}''$ moving on their way back to their original positions. And at time $d = b + (b - a)$ when they have arrived back we bring the $\psi_{\sigma'}''$ to rest by application of a final impulsive magnetic field gradient equal to the very first impulsive magnetic field gradient applied. (The 'rejected' functions $\psi_{\sigma'}$ (i.e. those with $\sigma' \notin \{\sigma_1, \dots, \sigma_n\}$) which were sent flying by the first applied magnetic impulse or by the scalar potential impulse) are by now so far away as to be unaffected by the final applied magnetic impulse.) The net result is to change the $\psi_{\sigma'}$ in (3.1.9) for $\sigma' \in \{\sigma_1, \dots, \sigma_n\}$ to $\psi_{\sigma'}^{iv}$ given by

$$\psi_{\sigma'}^{iv}(\mathbf{r}, t) = e^{-i\frac{\sigma'^2}{s^2}\mu^2k^2\delta^2(d-a)/2m\hbar} \psi_{\sigma'}(\mathbf{r}, t)$$

(cf. (1.6.2)). And we make $\psi_{\sigma'}^{iv}$ exactly the same as $\psi_{\sigma'}$ by choosing the value of $k\delta$ so that

$$\mu^2k^2\delta^2 \frac{d-a}{2m\hbar s^2} = 8\pi n \quad (3.1.11)$$

where n is an integer. Since σ' is an integer or half-integer the phase factor is then equal to 1 for all values of σ' .

To avoid significant natural evolution of $\psi_{\sigma'}(\mathbf{r}, t)$ for $\sigma' \in \{\sigma_1, \dots, \sigma_n\}$ during time $a < t < d$ we assume

$$d-a \ll \frac{2m}{\hbar} \Delta_{\psi_{\sigma'}}^2 \quad (3.1.12)$$

where $\Delta_{\psi_{\sigma'}}$ is the characteristic distance of spatial variation of $\psi_{\sigma'}(\mathbf{r}, t)$ (cf. (1.6.4)). Formally we should ideally let $d-a \rightarrow 0$ and $k\delta \rightarrow \infty$ while the displacement D' remains finite and large enough for separation. But we choose to keep $k\delta$ finite though extremely large.

Our measurement process is now effectively instantaneously carried out at time $t = a$, and after it (i.e. for $t > a$) the particle wave function is

$$\sum_{\sigma' \in \{\sigma_1, \dots, \sigma_n\}} \delta_{\sigma\sigma'} \psi_{\sigma'}(\mathbf{r}, t) + \sum_{\sigma' \notin \{\sigma_1, \dots, \sigma_n\}} \delta_{\sigma\sigma'} \psi'_{\sigma'}(\mathbf{r}, t)$$

where in the first summand the $\psi_{\sigma'}(\mathbf{r}, t)$ are the same as if we had left the particle alone, and in the second summand the $\psi'_{\sigma'}(\mathbf{r}, t)$ (for $\sigma' \neq 0$) are given by (3.1.8) and represent very fast moving wave packets set in motion by our first applied impulsive magnetic field gradient (or in case $\sigma' = 0$ a very fast moving wave packet set in motion by our applied impulsive scalar potential field gradient).

By the *law of motion under a part-quasi-classical wave function* the particle may be moving classically (to classical accuracy) as it would under one or other of the quasi-classical wave functions $\delta_{\sigma\sigma'} \psi'_{\sigma'}(\mathbf{r}, t)$ for one or other of the values of σ' outside the set $\{\sigma_1, \dots, \sigma_n\}$ (each of these motions being one with a definite spin component). And the modulus squared of the probability of this is

$$\sum_{\sigma' \notin \{\sigma_1, \dots, \sigma_n\}} \int |\psi'_{\sigma'}(\mathbf{r}, t)|^2 d^3\mathbf{r},$$

where the integral is over all space and the sum is restricted to values of σ' outside the set $\{\sigma_1, \dots, \sigma_n\}$. Such a motion would be directly observable and in the event that, by chance, no such motion is observed we learn that the particle must (just after time $t = a$) have been left behind in or returned to the region W of space, and therefore the point in configuration space (σ, \mathbf{r}) representing the particle motion must lie in the region of that space spanned by \mathbf{r} values in W and σ values in the set $\{\sigma_1, \dots, \sigma_n\}$. We can then restore the natural vector potential we temporarily removed and assuming we have not changed the values of particle coordinates \mathbf{r} and σ , we have achieved harmless conditioning in $S_\sigma S_r$. And by section 4 of Chapter II our wave function just after time $t = a$ is

$$\sum_{\sigma' \in \{\sigma_1, \dots, \sigma_n\}} \delta_{\sigma\sigma'} \psi_{\sigma'}(\mathbf{r}, a) K \tag{3.1.13}$$

with

$$K = \frac{e^{i\alpha}}{\sqrt{\sum_{\sigma' \in \{\sigma_1, \dots, \sigma_n\}} \int |\psi_{\sigma'}(\mathbf{r}, a)|^2 d^3\mathbf{r}}} \tag{3.1.14}$$

where α is an indeterminate constant phase.

To verify that our measurement does not in fact change the values of the particle coordinates \mathbf{r} and σ (i.e. to show that the propositions claiming values of these just before and just after our measurement imply one another with determinate phases), we suppose our initial wave function $\psi_{\sigma}(\mathbf{r}, t)$ is

$$\delta_{\sigma_1} \delta(\mathbf{r} - \mathbf{r}_1)$$

where \mathbf{r}_1 is a fixed point in region W and σ_1 a particular spin component. Or more exactly we consider a sequence of ordinary initial wave functions of the form $\psi_\sigma(\mathbf{r}, t) = \delta_{\sigma_1} \psi(\mathbf{r})$ that tend to $\delta_{\sigma_1} \delta(\mathbf{r} - \mathbf{r}_1)$. Then the procedure above for removing cases in which the spin component is outside any given set $\{\sigma_1, \dots, \sigma_n\}$ that includes σ_1 will leave any one of this sequence of ordinary wave functions unchanged and therefore it will leave the limiting wave function unchanged.* We deduce that the proposition ‘ $\sigma = \sigma_1, \mathbf{r} = \mathbf{r}_1$ ’ expressing our initial pure state of knowledge (together with the proposition representing our general knowledge) implies the truth of the proposition ‘ $\sigma = \sigma_1, \mathbf{r} = \mathbf{r}_1$ ’ immediately after the measurement, and it does so with a determinate phase of implication (namely zero). And by the general principle of reciprocity, the latter proposition implies the first with a determinate phase of implication (also zero). Propositions ‘ $\sigma = \sigma_1, \mathbf{r} = \mathbf{r}_1$ ’ just before and just after our measurement therefore claim correlated properties independently of our initial state of knowledge or whatever was our initial wave function $\psi_\sigma(\mathbf{r}, t)$.

We have thus successfully modelled a method which allows us at any time $t = a$ to perform instantly, in $S_\sigma S_r$, harmless conditioning with regard to a particle’s spin component. Just after successful application of the method our wave function $\psi_\sigma(\mathbf{r}, a)$ collapses to the form (3.1.13), or in case we seek to find the exact spin component σ_1 , to the form

$$\frac{e^{i\alpha} \delta_{\sigma_1} \psi_{\sigma_1}(\mathbf{r}, a)}{\sqrt{\int |\psi_{\sigma_1}(\mathbf{r}, a)|^2 d^3\mathbf{r}}} \quad (3.1.15)$$

where α is an indeterminate phase.

We finish by reviewing the conditions required for carrying out the above procedure of harmless conditioning with respect to the spin component. These are (3.1.10), (3.1.11) and (3.1.12). The first and last together are

$$s \frac{\mu k \delta}{\hbar} \Delta_\sigma < \frac{\mu^2 k^2 \delta^2 (b-a)}{m \hbar} \ll \frac{\mu^2 k^2 \delta^2}{\hbar^2} \Delta_{\psi_\sigma}^2 \quad (3.1.16)$$

which can clearly be satisfied by first choosing $b-a$ so that $(b-a)/m\hbar \ll \Delta_{\psi_\sigma}^2/\hbar^2$ and then making $k\delta$ sufficiently large. Then, since Δ_{ψ_σ} is less than or of the order of Δ_σ ,

* There are clearly no quasi-classical parts to the wave function moving out to infinity in these cases. Note also that in taking the limit (of $\delta_{\sigma_1} \psi(\mathbf{r})$ to $\delta_{\sigma_1} \delta(\mathbf{r} - \mathbf{r}_1)$) it will clearly be necessary to increase $k\delta$ indefinitely because the natural rate of change of initial wave functions in the sequence increases indefinitely.

(3.1.6) gives $\mu k \delta \Delta_\sigma / \hbar \gg s$ showing the middle term in (3.1.16) must certainly be large compared with s^2 so (3.1.11) can clearly be satisfied along with (3.1.10) and (3.1.12).

3.2 Simultaneous measurement of a particle's spin component and position

Finally we model a method for achieving, by chance, the simultaneous measurement of a particle's spin component and position at any time $t = a$.

Starting with a pure state of knowledge represented by a wave function $\psi_\sigma(\mathbf{r}, t)$ we first apply the method of section 3.1 to find, by chance, the spin component of the particle at time $t = a$. From the work in section 3.1 we see that, this leads (just after time $t = a$) to a collapsed wave function (in sample space $S_\sigma S_r$) of the form (3.1.15) which to within indeterminate phase factors separates into a wave function $\delta_{\sigma\sigma_1}$ in S_σ and a wave function $C_1 \psi_{\sigma_1}(\mathbf{r}, a)$ in S_r where

$$C_1 = \frac{e^{i\alpha}}{\sqrt{\int |\psi_{\sigma_1}(\mathbf{r}, a)|^2 d^3\mathbf{r}}}, \quad (3.2.1)$$

α being itself an indeterminate phase.

We next apply the method of section 2.1 by chance to further collapse the wave function $C_1 \psi_{\sigma_1}(\mathbf{r}, a)$ in S_r to

$$\begin{cases} C_2 C_1 \psi_{\sigma_1}(\mathbf{r}, a) & \mathbf{r} \in W_1 \\ 0 & \mathbf{r} \in W - W_1 \end{cases} \quad (3.2.2)$$

where

$$C_2 = \frac{e^{i\beta}}{\sqrt{\int_{W_1} |C_1 \psi_{\sigma_1}(\mathbf{r}, a)|^2 d^3\mathbf{r}}} \quad (3.2.3)$$

β being another indeterminate constant phase. Since our knowledge in S_σ and S_r remains separate during the second measurement process (the applied scalar potential having no effect on the spin component) our wave function in $S_\sigma S_r$ is now

$$\begin{cases} C \delta_{\sigma\sigma_1} \psi_{\sigma_1}(\mathbf{r}, a) & \mathbf{r} \in W_1 \\ 0 & \mathbf{r} \in W - W_1 \end{cases} \quad (3.2.4)$$

where $C = C_2 C_1$ and (as in section 2.1) the position of the particle cannot have been affected by the measurement.

We have thus achieved harmless conditioning in $S_\sigma S_r$. Taking W_1 to be arbitrarily small our collapsed wave function becomes simply

$$\delta_{\sigma\sigma_1} \delta(\mathbf{r}-\mathbf{r}_1) e^{i\beta} \quad (3.2.5)$$

where \mathbf{r}_1 is the location of the volume element $d^3\mathbf{r}$ to which W_1 has been reduced and β is an indeterminate constant phase, and we have achieved precise measurement of the particle's spin component and position without altering either.

All the above conclusions follow from the laws of quantum mechanics and complex-valued probability which therefore together confirm that instantaneous measurement of a particle's spin component and position by the method suggested above is both harmless with regard to position and spin component and *immediately repeatable* (i.e. reproducible) in principle.

3.3 The effect of measurement of one spin component on another

When we use the methods in sections 3.1 or 3.2 to harmlessly measure a particle's spin component in one particular fixed Cartesian coordinate system O we alter its spin component in any other coordinate system whose z axis lies on a different line through the origin of O , and alter it in an unpredictable way.

If for example we know initially the value of the z component σ' in coordinate system O' (whose z axis lies on a different line from the z axis of O) we cease to know the value of σ' in O' after measuring the value of σ in O . This is because the magnetic field H applied in the z direction of O to find the value of σ causes all spin components (in other coordinate systems) to undergo precession about the z axes of O at a rate $\mu H/s\hbar$ radians/unit time (as shown in section 8.3 of Chapter VII in the case of spin one-half) μ being the magnetic moment of the particle, s its spin and H the magnetic field at the point occupied by the particle at any stage of the measurement. After the first magnetic gradient impulse is applied the value σ' in O' is then the z component of spin in a coordinate system O'' which when rotated about the z axis of O through the angle $\Delta\phi = \mu H\delta/s\hbar$ coincides with O' . As a result the value of σ' in O' becomes uncertain because it is that which previously belonged to a coordinate system (namely O'') wherein the spin component was initially unknown.* Subsequent magnetic field impulses produce further uncertainties in σ' .

For things to be otherwise (e.g. for us to be able to maintain our knowledge of the value of σ' in O' in the above example) it would have to be that the angle $\Delta\phi$ whose order of magnitude is by (3.1.1)

* The magnitude of H and therefore of $\Delta\phi$ is also uncertain because of the uncertainty of the position of the particle in the high gradient of the magnetic field.

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$$\Delta\phi \approx \frac{\mu H}{s\hbar} \delta \approx \frac{\mu k \Delta}{s\hbar} \delta \quad (3.3.1)$$

(where Δ is the width of the region W in the x direction of O) was very small compared to 1, i.e. that

$$\frac{\mu k \Delta}{s\hbar} \delta \ll 1. \quad (3.3.2)$$

But this contradicts the necessary conditions for successful harmless measurement of σ in O as expressed in (3.1.10) and (3.1.12).

To confirm this contradiction we first note that when we initially know that σ' has value σ'_1 our initial wave function is of the form $\delta_{\sigma\sigma'_1} f(\mathbf{r})$ in O' and because of the separated form $\psi_\sigma(\mathbf{r}) = g(\sigma) f(\mathbf{r})$ of the corresponding initial wave function in O , the Δ_σ in (3.1.10) are all equal to Δ and the Δ_{ψ_σ} in (3.1.12) is a characteristic dimension of $f(\mathbf{r})$ and independent of σ' and accordingly we write it as Δ_f . So (3.1.10) and (3.1.12) are for present purposes

$$\frac{\mu}{s} k \delta \frac{b-a}{m} > \Delta \quad \text{and} \quad d-a \ll \frac{2m}{\hbar} \Delta_f^2 \quad (3.3.3)$$

where $d-a = 2(b-a)$. And since $\Delta_f \leq \Delta$ it easily follows from (3.3.3) that (3.3.2) cannot be fulfilled.

CHAPTER XIV

MIXED STATES OF KNOWLEDGE

With regard to an isolated quantum mechanical system in motion with known particle composition and known particle potentials*, the *pure* states of knowledge (of the system dynamics) considered so far are very special and only rarely arise in practice. Certain more general states of knowledge of the system dynamics are referred to as ‘mixed states’.[†] The representation of mixed states of knowledge by ‘arrays’ and the principles for assigning ‘arrays’ and for calculating probability distributions under mixed states of knowledge are given in the present Chapter XIV of the monograph. They have application of course to quantum statistical mechanics.

1. The representation of mixed states of knowledge

With regard to an isolated quantum mechanical system S with known particle composition and known particle potentials we know that a *pure state* of knowledge of the system dynamics is generally represented by a wave function $\Phi(x_i|Y)$ over a basis x_i ($i = 1, \dots, N$) in a sample space S (for S) covering a time period t_1 to t_2 , N being the dimension of all bases in S . (N is allowed to tend to infinity in certain cases but is taken as finite in the formulation of all basic theory— see section 3.1 of Chapter I.) A *mixed state* of knowledge of the system dynamics can be represented by a *set* of wave functions over a basis x_i with associated weights that add to one. Following Jaynes [20] we denote this as an ‘array’

$$\{\Phi(x_i|Y_1), \dots, \Phi(x_i|Y_m); w_1, \dots, w_m\} \quad (1.1)$$

where $\Phi(x_i|Y_j)$ ($j = 1, \dots, m$) are wave functions that would apply under generally different pure states of knowledge Y_j , and w_j ($j = 1, \dots, m$) are associated weights. The weights must always satisfy

$$w_j \geq 0, \quad \sum_{j=1}^m w_j = 1 \quad (1.2)$$

* We include the possibility that the particles move under the action of known *external* potentials as well as known inter-particle potentials. In saying the potentials are ‘known’ we mean of course that the *laws* of potential (the potentials as functions of particle positions and possibly the time) are known, not the actual values of the potentials.

[†] As in the case of pure states, the kinds of knowledge that constitute mixed states are learnt by experience.

In (1.1) the $\Phi(x_i|Y_j)$ ($j=1,\dots,m$) may be any (normalised) wave functions whatever, the weights w_j ($j=1,\dots,m$) may be any real numbers satisfying (1.2), and the number m of wave functions (or of their associated weights) may be any number from 1 to ∞ .^{*} Weight w_j is associated with wave function $\Phi(x_i|Y_j)$ and no other. (The wave functions $\Phi(x_i|Y_j)$ ($j=1,\dots,m$) need not form an orthogonal set or a complete set, they need not be linearly independent, and they may have indeterminate absolute phases.)

Law of equivalence of arrays

Two arrays represent the same mixed state of knowledge of system S dynamics if and only if their ‘density matrices’ with respect to the basis in question are equal[†], the density matrix for the general array (1.1) being defined as

$$\rho_{kn} = \sum_{j=1}^m w_j \Phi(x_k|Y_j) \Phi^*(x_n|Y_j) \quad (1.3)$$

A density matrix is evidently always a square matrix of size $N \times N$ where N is the dimension of all bases in the sample space S . It is also Hermitian, i.e. its transpose is equal to its conjugate:

$$\rho_{nk} = \rho_{kn}^* \quad (1.4)$$

The elements of a density matrix clearly have determinate amplitudes $|\rho_{kn}|$ and determinate absolute phases $\angle \rho_{kn}$ even if the wave functions themselves only have determinate relative phases. For if we multiply the $\Phi(x_k|Y_j)$ by $e^{i\alpha_j}$, the α_j being any constant (determinate or indeterminate) phases, we do not alter ρ_{kn} .

Law of equivalence of arrays (cont.)

If we take another basis y_p ($p=1,\dots,N$) in S (which may refer to the same time or to another time during the period t_1 to t_2 covered by S) an array in the y representation that represents the same mixed state as array (1.1) is

$$\{\Phi(y_p|Y_1), \dots, \Phi(y_p|Y_m); w_1, \dots, w_m\}$$

^{*} Any case in which the number of wave functions (or weights) is infinite can be dealt with by starting with m finite and taking the limit as $m \rightarrow \infty$. Certain sums, like those in (1.2) and (1.3), must then of course converge to finite values.

[†] We stress that equality of the density matrices is all that is required. We do not require the number of wave functions (or weights) in the corresponding arrays to be equal.

where the weights w_j ($j=1,\dots,m$) are the same as in (1.1) and the wave functions $\Phi(y_p|Y_j)$ ($j=1,\dots,m$) correspond to the same pure states of knowledge as the $\Phi(x_i|Y_j)$ and are therefore related to the latter by Feynman's law

$$\Phi(y_p|Y_j) = \sum_{i=1}^N \Phi(y_p|x_i)\Phi(x_i|Y_j). \quad (1.5)$$

Note however that the density matrix

$$\tilde{\rho}_{pq} = \sum_{j=1}^m w_j \Phi(y_p|Y_j)\Phi^*(y_q|Y_j)$$

in the y representation is not necessarily equal to the density matrix ρ_{kn} in the x representation. That is, a density matrix is (like a wave function) dependent on the representation.

Of course two arrays in the y representation represent the same mixed state of knowledge when their density matrices in the y representation are equal. And, for consistency, we require for two different sets of pure states Y_j ($j=1,\dots,m$) and Y'_j ($j'=1,\dots,m'$) and corresponding weights, that when

$$\sum_{j=1}^m w_j \Phi(y_p|Y_j)\Phi^*(y_q|Y_j) = \sum_{j'=1}^{m'} w'_{j'} \Phi(y_p|Y'_{j'})\Phi^*(y_q|Y'_{j'}) \quad (1.6)$$

we also have

$$\sum_{j=1}^m w_j \Phi(x_k|Y_j)\Phi^*(x_n|Y_j) = \sum_{j'=1}^{m'} w'_{j'} \Phi(x_k|Y'_{j'})\Phi^*(x_n|Y'_{j'}). \quad (1.7)$$

To show (1.7) follows from (1.6) we substitute (in (1.6)) for $\Phi(y_p|Y_j)$ and $\Phi(y_q|Y'_{j'})$ using (1.5) to get

$$\begin{aligned} & \sum_{i,i'} \sum_{j=1}^m w_j \Phi(y_p|x_i)\Phi(x_i|Y_j)\Phi^*(y_q|x_{i'})\Phi^*(x_{i'}|Y_j) \\ &= \sum_{i,i'} \sum_{j'=1}^{m'} w'_{j'} \Phi(y_p|x_i)\Phi(x_i|Y'_{j'})\Phi^*(y_q|x_{i'})\Phi^*(x_{i'}|Y'_{j'}) \end{aligned} \quad (1.8)$$

Here and henceforth we often omit (under summation signs) the limits of parameters like i and i' in (1.8), that run from 1 to N . By multiplying (1.8) through by

$\Phi(x_k|y_p)\Phi^*(x_n|y_q)$ and summing over p and q we change $\Phi(y_p|x_i)\Phi^*(y_q|x_i)$ to $\delta_{ik}\delta_{in}$, and obtain (1.7) as required.

A simple consequence of the first part of the law of equivalence of arrays is that if one of the weights of an array is zero, it, and its corresponding wave function can be removed from the array and it will serve just as well to present our mixed state of knowledge. Also any number of new weights (all equal to zero) may be included in an array, the new wave functions corresponding to them being chosen in any way we please.

Finally we note the following consequence of the second part of the law of equivalence of arrays. If the basis x_i employed in an array is taken to refer to a time dependent property (i.e. to be a time-dependent basis in our sample space S covering a time period), then a mixed state of knowledge represented by the array (1.1) and the mixed state of knowledge represented by the array

$$\{\Phi(x'_i|Y_1), \dots, \Phi(x'_i|Y_m); w_1, \dots, w_m\} \quad (1.9)$$

where the x'_i refer to the same property as the x_i but at a different time in the time period covered by S , are the same. This is because the wave functions $\Phi(x_i|Y_1)$ and $\Phi(x'_i|Y_1)$ are related by Feynman's law under the transformation functions $\Phi(x'_i|x_j)$, while the weights stay the same. We therefore have the following law:

Law of natural evolution of an array

Any array (1.1) whose basis is time-dependent represents the same mixed state of knowledge of a freely evolving (i.e. unmeasured) system if its wave functions evolve in time according to the Schrödinger equation while its weights remain the same.

2. The calculation of probabilities under mixed states of knowledge and the first law of array assignment. Knowledge relating to part of a system.

2.1 The calculation of probabilities under mixed states of knowledge

Under a mixed state of knowledge Z of a system S represented by an array of the form (1.1) the probabilities for the truth of propositions y_p ($p = 1, \dots, N$) of any basis y in our closed sample space S can be calculated from the following law.

The law of probabilities of the propositions of any basis

If our mixed state of knowledge Z is represented by array (1.1) using a basis x

then the probability we should assign to any one proposition y_p of a basis y in S is

$$\Phi(y_p|Z) = \sqrt{\sum_{j=1}^m w_j |\Phi(y_p|Y_j)|^2} e^{i\alpha_p} \quad (2.1.1)$$

the α_p ($p = 1, \dots, N$) being generally indeterminate and unrelated phases.

We also claim a law that gives the probabilities for different values of a dynamical property of S that may (among other things) be claimed by the propositions Y_j . As these values might be the same for two or more values of j , it is convenient to re-label the Y_j as Y_{nl} (and the w_j as w_{nl}) where parameters n and l may themselves (like j) stand for a number of parameters. So for each j there is a unique nl and vice versa. Now if the Y_{nl} claim property v_n (so that $Y_{nl'}$ with $l' \neq l$ also claims property v_n) then we have the following law.

Law of probabilities of parametric properties

If our mixed state of knowledge Z is represented by array $\{\dots, \Phi(x_i|Y_{nl}), \dots, w_{nl}, \dots\}$ and Y_{nl} claims (among other things) that dynamical variable v of S has value v_n then

$$\Phi(v_n|Z) = \sqrt{\sum_l w_{nl}} e^{i\beta_n} \quad (2.1.2)$$

where the β_n are phases generally indeterminate and unrelated for different n .

We stress that we do not require that the $\Phi(x_i|Y_{nl})$ be orthogonal and/or from a complete set of wave functions though this may sometimes be the case in applications. Law (2.1.2) holds quite generally.

The expected value of any function $f(v_n)$ of v_n is by definition

$$\bar{f} = \sum_n f(v_n) |\Phi(v_n|Z)|^2 \quad (2.1.3)$$

which by (2.1.2) is

$$\bar{f} = \sum_n \left(\sum_l f(v_n) w_{nl} \right) \quad (2.1.4)$$

where the range of values of parameter l may depend on the value of n .

The expected value of the deviation of f from its expected value \bar{f} , or the ‘standard deviation’ σ_f is defined as*

$$\sigma_f = \sqrt{(f - \bar{f})^2} = \sqrt{\sum_n (f(v_n) - \bar{f})^2 |\Phi(v_n|Z)|^2} \quad (2.1.5)$$

and is accordingly given by

$$\sigma_f = \sqrt{\sum_n \left(\sum_l (f(v_n) - \bar{f})^2 w_{nl} \right)}. \quad (2.1.6)$$

2.2 The first law of array assignment

To help us establish arrays of the form (1.1) for representing mixed states of knowledge of an isolated system S to which our closed sample space S refers (with the x_i forming a basis in S) we have laws of array assignment that play a role similar to the principles of probability assignment employed in connection with wave functions representing pure states. We give below the first of the laws relating to array assignment.

First law of array assignment

Whenever we could if we wished acquire (harmlessly with respect to any proposition in S), one of a certain set of pure states of knowledge Y_j ($j=1, \dots, m$) of S , and our degrees of belief π_j ($j=1, \dots, m$) for acquiring one or other of the states of knowledge Y_j ($j=1, \dots, m$) are known to us, we are in a mixed state of knowledge (with respect to the propositions of S) represented by array (1.1) with $w_j = \pi_j$ ($j=1, \dots, m$). And taking this array to represent our (mixed) state of knowledge, knowledge of the possibility of harmless acquisition of one or other of the pure states of knowledge Y_j etc. becomes redundant as far as our knowledge of the system dynamics itself is concerned.†

* Note that whenever we employ the term ‘expected value’ (e.g. ‘expected energy’, ...etc.) we mean of course the *probabilistic average* and ‘expectation’ here bears no relation to the *logical expectation* associated with propositions whose probabilities have unit moduli and indeterminate phases (section 2.2.2 of Chapter I).

† We stress that the converse of the first law of array assignment is *not* true. That is, holding a mixed state of knowledge of a system’s dynamics represented by an array $\{\Phi(y_p|Y_1), \dots, \Phi(y_p|Y_m); w_1, \dots, w_m\}$ does

Now in order to be able to acquire harmlessly with respect to any proposition of S , one or other of a set of pure states of knowledge Y_j ($j=1,\dots,m$) of S it is necessary that information in the form of observable macroscopic states of matter be available to us for the purpose of determining *which* pure state of knowledge to adopt. This is the case if, for example, somebody else tells us they have prepared the system S so that, with regard to it, they themselves are in a one or other pure state of knowledge Y_j ($j=1,\dots,m$) without telling us which. If we are able to calculate a degree of belief π_j ($j=1,\dots,m$) for each possible choice of that person, then (by the first law of array assignment) we are in a mixed state of knowledge represented by (1.1) with weights $w_j = \pi_j$ ($j=1,\dots,m$). Harmless acquisition by us of a *pure* state of knowledge Y_j could then be simply achieved (if we so wished) by asking the other person which choice they made.

When the first law of array assignment applies there is a simple way to calculate a degree of belief distribution over the propositions x_i of basis x in S which agrees with the law of probabilities of the propositions of any basis (section 2.1). Under our mixed state of knowledge Z our degree of belief in any of the propositions x_i of the basis x in S , may now be calculated using the sum rule (2.3.2) of Chapter I and the product rule (2.4.1) of Chapter I. We have by the sum rule that

$$|\Phi(x_i|Z)|^2 = |\Phi(x_i(Y_1 + \dots + Y_m)|Z)|^2 = |\Phi(x_i Y_1 + \dots + x_i Y_m|Z)|^2 = |\Phi(x_i Y_1|Z)|^2 + \dots + |\Phi(x_i Y_m|Z)|^2 \dots(2.2.1)$$

The product rule $\Phi(x_i Y_j|Z) = \Phi(Y_j|Z)\Phi(x_i|Y_j Z)e^{i(k+\epsilon_j)}$ where k and ϵ_j are respectively phases characteristic of knowledge Z and Y_j , applies for $j=1,\dots,m$ because it is possible in principle (in our special case) to acquire knowledge of Y_j (or its equivalent) harmlessly with respect to S so x_i and Y_j are compatible. Putting $|\Phi(Y_j|Z)|^2 = \pi_j$ and $w_j = \pi_j$, and noting that Z is redundant in $\Phi(x_i|Y_j Z)$ we find from (2.2.1) that

$$|\Phi(x_i|Z)|^2 = \sum_{j=1}^m w_j |\Phi(x_i|Y_j)|^2 \quad (2.2.2)$$

in agreement with the general rule (2.1.1). We likewise easily find agreement with (2.1.2).

not in itself imply the possibility of getting to know harmlessly which state of pure knowledge Y_j we can adopt.

2.3 The case of a pure state

We claim (as part of our general knowledge) that a mixed state of system dynamics is also a pure state if and only if it can be represented by an array of the form (1.1) in which the wave functions associated with the non-zero weights (say n in number, with of course $1 \leq n \leq m$) are all the same –all say $\Phi(x_i|Y)$. A ‘pure state’ array thus takes the form

$$\left\{ \Phi(x_i|Y_1), \dots, \Phi(x_i|Y_{p-1}), \Phi(x_i|Y), \dots, \Phi(x_i|Y), \Phi(x_i|Y_{p+n}), \dots, \Phi(x_i|Y_m); 0, \dots, 0, w_p, \dots, w_{p+n-1}, 0, \dots, 0 \right\} \quad \dots(2.3.1)$$

where the equal wave functions (and their weights) are grouped together for convenience.

By the first law of array assignment, if we knew that the p^{th} wave function $\Phi(x_i|Y)$ in a set of n identical wave functions should apply with degree of belief w_p , and other wave functions ($m - n$ in number) should apply with degree of belief zero, then our total degree of belief in the wave function $\Phi(x_i|Y)$ applying would be $w_p + \dots + w_{p+n-1} = 1$. And this is consistent with the claim that (2.3.1) represents a pure state of knowledge.

The density matrix for (2.3.1) is clearly

$$\rho_{km} = \sum_{j=p}^{p+n-1} w_j \Phi(x_k|Y) \Phi^*(x_n|Y) = \Phi(x_k|Y) \Phi^*(x_n|Y) \quad (2.3.2)$$

and since arrays with the same density matrix in the same representation represent the same mixed state of knowledge we can say, for example, that an array of the form

$$\left\{ \Phi(x_i|Y_1), \dots, \Phi(x_i|Y_m); 0, \dots, 0, 1, 0, \dots, 0 \right\} \quad (2.3.3)$$

in which all but one (say the p^{th}) weight is zero represents a pure state of knowledge with wave function $\Phi(x_i|Y_p)$. When we consider mixed states represented by arrays in which the wave functions $\Phi(x_i|Y_j)$ ($j = 1, \dots, m$) are a certain set of orthogonal wave functions forming a complete set, these mixed states can clearly only be pure states when all but one of the weights is zero (as in (2.3.3)).

2.4 The case of knowledge relating to part of a system

In section 8 of Chapter II we gave an example of a mixed state of knowledge. This related to knowledge regarding a part of a system when knowledge of the whole system was pure. The connection between the observations of section 8 of Chapter II and the work of the present section is as follows.

As in section 8 of Chapter II, suppose $S^{(1)}$ (of order N_1) and $S^{(2)}$ (of order N_2) are contemporary and complete sample spaces of propositions about the dynamical properties of non-interacting systems $S^{(1)}$ and $S^{(2)}$ respectively, and suppose basis $x_i^{(1)}$ and primary basis $x_j^{(2)}$ are bases in $S^{(1)}$ and $S^{(2)}$ respectively pertaining to the same time t . Using basis $x_i^{(1)}x_j^{(2)}$ in $S^{(1)}S^{(2)}$, let our wave function, under knowledge Y (pure and inseparable in relation to the sample space $S^{(1)}S^{(2)}$ of the whole system) be $\Phi(x_i^{(1)}x_j^{(2)}|Y)$.

Let $y_k^{(1)}$ be a primary basis in $S^{(1)}$, then (see section 7 of Chapter II) the moduli of the probabilities $\Phi(y_k^{(1)}|Y)$ are calculable and there is the possibility that we could, harmlessly with respect to $S^{(2)}$, by chance acquire knowledge that $y_k^{(1)}$ was true, after which our wave function in $S^{(2)}$ would be $\Phi(x_i^{(2)}|y_k^{(1)}Y)$ which is also calculable (see section 7 of Chapter II). We claim that under knowledge Y of the whole system $S^{(1)}S^{(2)}$ we are in a mixed state of knowledge regarding the dynamical properties of the system $S^{(2)}$, and an array representing our mixed state of knowledge with regard to $S^{(2)}$ is

$$\left\{ \dots, \Phi(x_j^{(2)}|y_k^{(1)}Y), \dots; \dots, |\Phi(y_k^{(1)}|Y)|^2, \dots \right\} \quad (2.4.1)$$

i.e. the array of wave functions $\Phi(x_i^{(2)}|y_k^{(1)}Y)$ $k=1, \dots, N_1$ with associated weights $|\Phi(y_k^{(1)}|Y)|^2$.*

The formula

$$\Phi(x_j^{(2)}|Y) = \sqrt{\sum_k |\Phi(y_k^{(1)}|Y)\Phi(x_j^{(2)}|y_k^{(1)}Y)|^2} e^{i\alpha_j}$$

derived in section 8 of Chapter II, for the probability distribution over the $x_j^{(2)}$ given Y , is (as required) in agreement with the general law (2.1.1) (applied to (2.4.1)) for calculating the probability distribution over the basis employed in an array representing a mixed state of knowledge.

3. The product rule for arrays

In analogy with the product rule for wave functions under pure states of knowledge (section 3.7 of Chapter I) we assume the truth of the following product rule for arrays.

* Note that, although we can *by chance* acquire knowledge that $y_k^{(1)}$ is true, we cannot acquire this knowledge *on demand*, so it does not automatically follow that (under knowledge Y) we are in a mixed state of knowledge with regard to $S^{(2)}$. But we can (and do) claim we are.

Let $S^{(1)}$ and $S^{(2)}$ be two quantum mechanical systems or distinct aspects of one system and let their properties be referred respectively to separately closed sample spaces $S^{(1)}$ and $S^{(2)}$.

If $Z^{(1)}$ is our mixed state of knowledge of system $S^{(1)}$ in relation to sample space $S^{(1)}$ and $Z^{(2)}$ is our mixed state of knowledge of system $S^{(2)}$ in relation to sample space $S^{(2)}$, and if $S^{(1)}$ and $S^{(2)}$ are known (or assumed to be) *logically independent* under knowledge $Z^{(1)}Z^{(2)*}$, then $Z^{(1)}Z^{(2)}$ is a mixed state of knowledge of the combined system $S^{(1)}S^{(2)}$ in relation to the combined sample space $S^{(1)}S^{(2)}$. And if

$$\left\{ \Phi(x_i^{(1)}|Y_1^{(1)}), \dots, \Phi(x_i^{(1)}|Y_{m_1}^{(1)}); w_1^{(1)}, \dots, w_{m_1}^{(1)} \right\} \quad (3.1)$$

and

$$\left\{ \Phi(x_i^{(2)}|Y_1^{(2)}), \dots, \Phi(x_i^{(2)}|Y_{m_2}^{(2)}); w_1^{(2)}, \dots, w_{m_2}^{(2)} \right\} \quad (3.2)$$

are arrays representing our mixed states of knowledge $Z^{(1)}$ and $Z^{(2)}$ respectively, an array representing our mixed state of knowledge $Z^{(1)}Z^{(2)}$ is relation to $S^{(1)}S^{(2)}$ is

$$\left\{ \dots, \Phi(x_i^{(1)}|Y_p^{(1)})\Phi(x_j^{(2)}|Y_q^{(2)}), \dots; \dots, w_p^{(1)}w_q^{(2)}, \dots \right\} \quad (3.3)$$

where p and q take all possible values (from 1 to m_1 in the case of p and from 1 to m_2 in the case of q). Clearly the weights $w_p^{(1)}w_q^{(2)}$ in array (3.3) satisfy the conditions

$$\sum_{p=1}^{m_1} \sum_{q=1}^{m_2} w_p^{(1)}w_q^{(2)} = 1$$

$$w_p^{(1)}w_q^{(2)} \geq 0,$$

required of any array. We call (3.3) the *product rule for arrays*.

The density matrices going with arrays (3.1) to (3.3) are

$$\rho_{kn}^{(1)} = \sum_{p=1}^{m_1} w_p^{(1)} \Phi(x_k^{(1)}|Y_p^{(1)}) \Phi^*(x_n^{(1)}|Y_p^{(1)}), \quad (3.4)$$

$$\rho_{rs}^{(2)} = \sum_{q=1}^{m_2} w_q^{(2)} \Phi(x_r^{(2)}|Y_q^{(2)}) \Phi^*(x_s^{(2)}|Y_q^{(2)}), \quad (3.5)$$

$$\rho_{knrs} = \sum_{p=1}^{m_1} \sum_{q=1}^{m_2} w_p^{(1)}w_q^{(2)} \Phi(x_k^{(1)}|Y_p^{(1)}) \Phi(x_n^{(2)}|Y_q^{(2)}) \cdot \Phi^*(x_r^{(1)}|Y_p^{(1)}) \Phi^*(x_s^{(2)}|Y_q^{(2)}). \quad (3.6)$$

* Note that there is no law (like the law of absolute logical independence under pure knowledge) that would make $S^{(1)}$ and $S^{(2)}$ *necessarily* logically independent.

and we note that

$$\rho_{knrs} = \rho_{kr}^{(1)} \rho_{ns}^{(2)}. \quad (3.7)$$

Conversely, if in relation to the combination $S^{(1)}S^{(2)}$ of separately closed sample spaces $S^{(1)}$ and $S^{(2)}$ we have a mixed state of knowledge represented by an array of the (factorized) form (3.3)* over basis $x_i^{(1)}x_j^{(2)}$ of $S^{(1)}S^{(2)}$, and therefore one whose density matrix ρ_{knrs} factors as in (3.7), then our knowledge separates into logically independent mixed states of knowledge $Z^{(1)}$ and $Z^{(2)}$ in relation to $S^{(1)}$ and $S^{(2)}$ respectively represented by arrays (3.1) and (3.2).

4. Diagonalisation of the density matrix and the law of orthogonal representation of mixed states of knowledge

Any square Hermitian matrix (and therefore the general density matrix ρ_{kn} in (1.3)) can be diagonalised by means of a unitary transformation (see for example chapter 10 of [10]). So for any density matrix ρ with elements ρ_{kn} a unitary matrix U with elements U_{pk} and inverse U^{-1} with elements $(U^{-1})_{nq} = U_{nq}^{-1}$ can always be found such that

$$\sum_{kn} U_{pk} \rho_{kn} U_{nq}^{-1} = d_{pq} = d_p \delta_{pq} \quad (4.1)$$

where d_{pq} is a diagonal matrix with diagonal elements d_p .

From (4.1) we have

$$\sum_{knp} U_{lp}^{-1} U_{pk} \rho_{kn} U_{nq}^{-1} = \sum_p d_p \delta_{pq} U_{lp}^{-1}$$

or

$$\sum_n \rho_{ln} U_{nq}^{-1} = d_q U_{lq}^{-1}. \quad (4.2)$$

So the columns $q = 1, \dots, N$ of U_{nq}^{-1} are eigenvectors of ρ_{ln} with eigenvalues d_q .

By (4.1)

* Of course, if the weights w_{pq} of an array over basis $x_i^{(1)}x_j^{(2)}$ factor as in (3.3) they can only factor in one way. For if $w_{pq} = w_p^{(1)}w_q^{(2)} = w_p^{\prime(1)}w_q^{\prime(2)}$ for all p and q , then by summing $w_p^{(1)}w_q^{(2)} = w_p^{\prime(1)}w_q^{\prime(2)}$ over say q we obtain $w_p^{(1)} = w_p^{\prime(1)}$ for all p .

$$\sum_{nl} U_{ql} \rho_{ln} U_{nq}^{-1} = d_q \quad (4.3)$$

Substituting for ρ_{ln} using (1.3) we get

$$\sum_{j=1}^m w_j \sum_{nl} U_{ql} \Phi(x_l | Y_j) \Phi^*(x_n | Y_j) U_{nq}^{-1} = d_q \quad (4.4)$$

or

$$\sum_{j=1}^m w_j \sum_l U_{ql} \Phi(x_l | Y_j) \sum_n U_{nq}^{-1} \Phi^*(x_n | Y_j) = d_q .$$

Here, by the unitary property

$$U_{nq}^{-1} = U_{qn}^* \quad (4.5)$$

the sum over n is the conjugate of the sum over l so

$$\sum_{j=1}^m w_j \left| \sum_l U_{ql} \Phi(x_l | Y_j) \right|^2 = d_q$$

showing that

$$d_q \geq 0 \quad (4.6)$$

for all q . Also summing (4.4) over q gives

$$\sum_{j=1}^m w_j \sum_{nl} \delta_{nl} \Phi(x_l | Y_j) \Phi^*(x_n | Y_j) = \sum_q d_q$$

and since the $\Phi(x_l | Y_j)$ are normalised and the w_j add to 1 we have

$$\sum_q d_q = 1. \quad (4.7)$$

Now the eigenvector columns of U_{nq}^{-1} in (4.2) can be used to define N new wave functions $\Phi(x_k | Y'_p)$ under new pure states of knowledge Y'_p . Thus we put

$$U_{kp}^{-1} = \Phi(x_k|Y'_p)e^{-i\alpha_p} \quad \text{or} \quad U_{pk} = \Phi^*(x_k|Y'_p)e^{i\alpha_p} \quad (4.8)$$

where the Y'_p are the pure states of knowledge that would result in wave functions $\Phi(x_k|Y'_p)$ equal to U_{kp}^{-1} multiplied by a phase factor $e^{i\alpha_p}$ independent of k . The unitary property of U makes the wave functions orthonormal because

$$\delta_{pq} = \sum_k U_{pk}U_{kq}^{-1} = \sum_k U_{pk}U_{qk}^* = \sum_k \Phi^*(x_k|Y'_q)\Phi(x_k|Y'_p) \quad (4.9)$$

Also the array

$$\{\Phi(x_i|Y'_1), \dots, \Phi(x_i|Y'_N); d_1, \dots, d_N\} \quad (4.10)$$

of the new wave functions with respective weights equal to the diagonal elements of the diagonalised density matrix has a density matrix ρ'_{kn} equal to the original density matrix ρ_{kn} . For

$$\rho'_{kn} = \sum_p d_p \Phi(x_k|Y'_p)\Phi^*(x_n|Y'_p)$$

which, using (4.1), can be written (with harmless inclusion of a factor $e^{-i(\alpha_p - \alpha_q)}$ in the summand) as

$$\rho'_{kn} = \sum_{qp} d_q \delta_{pq} e^{-i(\alpha_p - \alpha_q)} \Phi(x_k|Y'_p)\Phi^*(x_n|Y'_q) = \sum_{qpkn'} U_{pk'}\rho_{k'n'}U_{n'q}^{-1}\Phi(x_k|Y'_p)e^{-i\alpha_p}\Phi^*(x_n|Y'_q)e^{i\alpha_q} \dots(4.11)$$

And by (4.8) this is

$$\rho'_{kn} = \sum_{qpkn'} U_{pk'}\rho_{k'n'}U_{n'q}^{-1}U_{pk}^*U_{qn} \quad (4.12)$$

in which

$$\sum_q U_{n'q}^{-1}U_{qn} = \delta_{nn'}, \quad \sum_p U_{pk'}U_{pk}^* = \delta_{kk'},$$

giving $\rho'_{kn} = \rho_{kn}$.

Hence array (4.10) represents the same mixed state of knowledge as array (1.1). And there follows the general possibility of 'orthogonal representation' of any mixed state of knowledge in relation to any closed sample space S :

Law of orthogonal representation of mixed states of knowledge

A mixed state of knowledge of the dynamical properties of an isolated quantum mechanical system can always be represented by an array of N *orthogonal* wave functions with associated weights, N being the dimension of bases in the sample space S or the order of the sample space S .

Note well, however, that the N orthogonal wave functions mentioned in this law cannot be just *any* N orthogonal wave functions of our choice. They are generally dependent on the mixed state in question.

Being the eigenvalues of the matrix ρ_{kn} , the d_q ($q=1,\dots,N$) are always the same set of numbers no matter what unitary transformation U is used to diagonalise ρ_{kn} , but the orthogonal functions $\Phi(x_i|Y'_q)$ with which they are associated in (4.10) are not always the same. If (and only if) there is degeneracy of the d_q values (i.e. if some are the same as others) there is more than one unitary matrix U that will diagonalise ρ_{kn} and each will give rise to a different set of orthonormal functions $\Phi(x_i|Y'_q)$. The density matrix ρ'_{kn} is however not affected by this freedom in the choice of the diagonalising unitary transformation. As we have demonstrated ρ'_{kn} always remains the same as the original density matrix ρ_{kn} .

As a consequence of the existence of more than one unitary transformation in the case of degeneracy of the d_q values, we are at liberty (without changing the d_q values) to replace the mutually orthogonal wave functions $\Phi(x_i|Y'_q)$ for any set of q values for which d_q are equal, by any other set of mutually orthogonal wave functions that remain orthogonal to the wave functions $\Phi(x_i|Y'_q)$ for all *other* q values.

To show this explicitly, suppose the first r values of the d_q in (4.10) are equal and let us perform a unitary transformation $U_{qq'}$ taking the orthogonal wave functions $\Phi(x_i|Y'_q)$ for $q=1,\dots,r$ to new orthogonal wave functions for $q=1,\dots,r$ while leaving the remaining $\Phi(x_i|Y'_q)$ the same. That, is let

$$\Phi(x_i|\tilde{Y}'_q) = \begin{cases} \sum_{q'=1}^r U_{qq'} \Phi(x_i|Y'_{q'}) & q=1,\dots,r \\ \Phi(x_i|Y'_q) & q=r+1,\dots,N \end{cases} \quad (4.13)$$

where the $r \times r$ square matrix $U_{qq'}$ is unitary. With the same weights this new set of wave functions gives the density matrix

$$\tilde{\rho}_{kn} = \sum_q d_q \Phi(x_k|\tilde{Y}'_q) \Phi^*(x_n|\tilde{Y}'_q).$$

This will clearly be the same as the original density matrix if

$$\sum_{q=1}^r \Phi(x_k | \tilde{Y}_q) \Phi^*(x_n | \tilde{Y}_q) = \sum_{q=1}^r \Phi(x_k | Y'_q) \Phi^*(x_n | Y'_q) \quad (4.14)$$

but this is evidently the case because on substituting for the $\Phi(x_i | \tilde{Y}_q)$ using (4.13) we get for the LHS of (4.12)

$$\sum_{q=1}^r \sum_{q'=1}^r U_{qq'} \Phi(x_k | Y'_{q'}) \sum_{q''=1}^r U_{qq''}^* \Phi^*(x_n | Y'_{q''})$$

which reduces to the RHS of (4.14) on account of the unitary property of $U_{qq'}$ that makes

$$\sum_{q=1}^r U_{qq'} U_{qq''}^* = \sum_{q=1}^r U_{qq'} U_{q''q}^{-1} = \delta_{q'q''}.$$

The transformation (4.13) is equivalent to a transformation of the ‘vector’ of all the N wave functions by a $N \times N$ unitary matrix $U_{qq'}$ whose elements are, for $q = 1, \dots, r$ and $q' = 1, \dots, r$ identical to those used above, and for other values of q and q' are equal to $\delta_{qq'}$. We can clearly make, in succession, unitary transformations that ‘rotate together’ in any way we please the wave functions associated with each set of q values for which the d_q have the same value. The result will be a net unitary transformation of the vector of the original set of N orthogonal wave functions by means of a $N \times N$ unitary matrix. And so in connection with the above law of orthogonal representation of a mixed state of knowledge we have the following law of equivalence:

Law of equivalence of orthogonal representations of a mixed state of knowledge

If, in an orthogonal representation of a mixed state of knowledge the wave functions fall into sets each associated with weights of equal value, it will make no difference to the density matrix, nor invalidate the representation of our mixed state of knowledge, if we apply a unitary transformation to the wave functions that ‘rotates together’ in an arbitrary manner the wave functions of each set independently.

5. The second law of array assignment or the method of maximum entropy

When we have a pure state of knowledge about the dynamical properties of a quantum mechanical system we are, as we have said before, on the boundary of possible knowledge under the uncertainty principle. Under a mixed state of knowledge about the

dynamical properties of a quantum mechanical system our knowledge generally falls short of being pure. The degree to which it falls short, i.e. the amount of our ignorance of the dynamical properties over and above the natural limits imposed by the uncertainty principle is axiomatically measured by a real number S called the ‘information entropy’ or the ‘entropy’ for short. And this ‘entropy’ is calculated as follows (Jaynes [20]).

Let our mixed state of knowledge be represented by an array of the form (1.1). To calculate the information entropy for this state of knowledge we start by applying the method of section 4 to obtain an array (4.10) of N orthogonal wave functions with the same density matrix. As we have said before, although there may be more than one unitary transformation for carrying out the procedure in section 4, the resulting weights d_1, \dots, d_N in the new array are always the same, being, as they are, the eigenvalues of the original density matrix. Only the wave functions with which they are associated may differ (in the case of degeneracy). In terms of the set of d_i values whatever they may be, the information entropy is

$$S = -\sum_{i=1}^N d_i \ln d_i \quad (5.1)$$

it being understood that if one of the d_i values (say d_j) is zero the value of the summand for $i = j$ is zero.

In the case of a pure state of knowledge all the d_i values must be zero except one (as in (2.3.3)), and the value of S is accordingly zero. This is clearly the minimum value the information entropy can take.

The maximum value that S can take is found by maximising the RHS of (5.1) subject to the constraint (4.7). That is, following Lagrange, we maximise

$$L = -\sum_{i=1}^N d_i \ln d_i + \lambda \sum_i d_i$$

subject to no constraint and then fix the constant λ by imposing the condition (4.7). This gives

$$d_i = \frac{1}{N}$$

and so

$$S_{\max} = -\sum_{i=1}^N \frac{1}{N} \ln \frac{1}{N} = \ln N. \quad (5.2)$$

That is, the maximum possible value of the information entropy is the natural logarithm of the dimension of bases in the sample space. This is the value of the information

entropy that applies when we are completely ignorant of the dynamical properties of the quantum mechanical system (see section 6).

The second law of array assignment or the method of maximum entropy can now be stated as follows.

Second law of array assignment or the method of maximum entropy

With regard to an isolated quantum mechanical system with known particle composition and known particle potentials, if our mixed knowledge regarding dynamical properties of the system can be expressed as constraints imposed upon the unknown weights d_1, \dots, d_N in a representative array of N known orthogonal wave functions, then the values of the weights can be found by maximising the information entropy $S = -\sum_{i=1}^N d_i \ln d_i$ subject to the constraints.

Like the method of maximum entropy in classical probability theory the second law of array assignment is a natural consequence of the assumption that information entropy measures the amount of ignorance. To assign values to the d_1, \dots, d_N that satisfy the (known) constraints but do *not* maximise S would be to claim to know more about the system dynamics than we actually do.

6. Case of complete ignorance of dynamical properties and the third law of array assignment

Let the dynamical properties of a quantum mechanical system S be represented by propositions in a closed sample space S of order N . In connection with the case of complete ignorance of the dynamical properties we introduce a third law of array assignment which extends the principle of indifference (section 5.2 of Chapter I):

Third law of array assignment If we are totally ignorant of the dynamical properties of the system, our state of knowledge is mixed and can be represented by an array of *any* set of N orthogonal (allowed) wave functions with *equal* weights associated with each.*

The weights are then, by (1.2) simply

* Note that, when we are ‘totally ignorant’ of the dynamical properties of a system, we suppose we still have knowledge of the *unchanging* properties of that system, e.g. knowledge of the system potential function. And that knowledge may imply certain limited knowledge of the system dynamics. For example, for a single particle system, if we know the potential field it moves in is infinite in a certain region of space, then we know the particle cannot be in that region. But the third law of array assignment can still be taken to apply in such cases provided we understand that the N orthogonal wave functions are *allowed* wave functions, i.e. wave functions that are allowed when we take into account our knowledge of the unchanging properties of the system. So in the single particle example, any set of orthogonal wave functions in the particle position representation must be wave functions that vanish within the region of infinite potential.

$$w_j = \frac{1}{N} . \quad (6.1)$$

To prove consistency of this third law we need to show that the resulting density matrix

$$\rho_{kn} = \sum_{j=1}^N \frac{1}{N} \Phi(x_k|Y_j)\Phi^*(x_n|Y_j) \quad (6.2)$$

is the same for any orthogonal set of wave functions $\Phi(x_k|Y_j)$ $j=1,\dots,N$. Letting the wave functions be represented by a matrix A with elements A_{kj} given by

$$\Phi(x_k|Y_j) = A_{kj}$$

the orthogonality of the wave functions gives

$$\sum_k A_{kj} A_{kj'}^* = \delta_{jj'}$$

showing that

$$A_{kj}^* = (A^{-1})_{jk} = A_{jk}^{-1}$$

and therefore, by (6.2),

$$\rho_{kn} = \sum_j \frac{1}{N} A_{kj} A_{jn}^{-1} = \frac{1}{N} \delta_{kn} . \quad (6.3)$$

So the density matrix is just $1/N$ times the unit matrix and must therefore be the same whatever set of orthogonal wave functions $\Phi(x_k|Y_j)$ is chosen.

Taking the orthogonal wave functions to be $\Phi(x_k|Y_j) = \delta_{kj}$ (corresponding to pure states of knowledge $Y_j = x_j$ ($j=1,\dots,N$)) we find, from the general result (2.1.1), that under a state of knowledge Z representing complete ignorance of the dynamical properties of the system,

$$|\Phi(x_i|Z)|^2 = \sum_{j=1}^N \frac{1}{N} |\delta_{ij}|^2 = \frac{1}{N} . \quad (6.4)$$

So the probabilities for the truth of the propositions x_i ($i=1,\dots,N$) of any basis x in our sample space each have moduli $\frac{1}{\sqrt{N}}$ and indeterminate phases.

Consider any set of pure states of knowledge Y_j ($j=1,\dots,N$), the wave functions $\Phi(x_k|Y_j)$ of which form an orthogonal set. By the law of inferred dynamical properties (section 3.11 of Chapter I), knowledge Y_j amounts to knowledge that the value of a (generally inferred) property P of the system is quantified by j (or that property P_j applies). In the (mixed) state of complete ignorance of the dynamical properties of the system we thus assign equal weights to each possible value j of property P .

As a simple example, suppose we are given an isolated spin one-half particle and have no information whatsoever about its component of spin in any direction. Then with regard to its spinning motion we are in a mixed state of knowledge which can be represented by the array

$$\left\{ \Phi(\sigma|\frac{1}{2}), \Phi(\sigma|-\frac{1}{2}); \frac{1}{2}, \frac{1}{2} \right\} \quad (6.5)$$

where the wave functions are functions of the z component of spin σ in any one fixed Cartesian coordinate system O under pure states of knowledge $\sigma' = \frac{1}{2}$ and $\sigma' = -\frac{1}{2}$ in another fixed Cartesian coordinate system O' . That is, the wave functions in (6.5) are the transformation functions $\Phi(\sigma|\sigma')$ for $\sigma' = \frac{1}{2}$ and $\sigma' = -\frac{1}{2}$, and are of course necessarily orthogonal to each other. Our density matrix is therefore the 2×2 matrix

$$\rho_{kn} = \frac{1}{2} \left(\Phi(\sigma_k|\frac{1}{2})\Phi^*(\sigma_n|\frac{1}{2}) + \Phi(\sigma_k|-\frac{1}{2})\Phi^*(\sigma_n|-\frac{1}{2}) \right) \quad (6.6)$$

where the σ_k ($k=1,2$) stand respectively for spin components $\sigma = \frac{1}{2}$ and $\sigma = -\frac{1}{2}$ in O and the σ_n ($n=1,2$) also stand respectively for spin components $\sigma = \frac{1}{2}$ and $\sigma = -\frac{1}{2}$ in O' . By the formulae for the transformation functions for spin one-half (Chapter VII) the RHS of (6.6) equals $\frac{1}{2}\delta_{kn}$ in agreement with (6.3). To the proposition claiming the z component of spin σ in O is $1/2$, we should assign (by (6.4)) a probability of modulus $1/\sqrt{2}$ and indeterminate phase.

We note that, by the first law of array assignment, our state of knowledge regarding the particle spin is in this example the same as it would be if we were told somebody else had prepared the particle with a definite component σ' of spin relative to a specified fixed Cartesian coordinate system O' without revealing whether σ' was $\frac{1}{2}$ or $-\frac{1}{2}$. By the principle of indifference we would then calculate a degree of belief of $\frac{1}{2}$ for each possible choice of that person and hence form the array (6.5). But in the absence of any knowledge about the spinning motion we should anyway form array (6.5) to represent our knowledge. And if we were then to acquire the above knowledge regarding

the preparation of a definite spin component by someone else, this new knowledge would be quite redundant as far as our knowledge of the spinning motion itself was concerned. It would add nothing to that knowledge. The ‘new’ knowledge would take different forms depending on the particular coordinate system O' revealed to us by the other person. Different pure states would have been prepared in each case but our knowledge of the spinning properties of the particle would remain the same. We note this would be difficult to understand if pure states were taken to be *physical states of the system* rather than *states of our knowledge of the system*.

7. The fourth law of array assignment

We introduce a fourth law of array assignment which extends the principle of similarity (sections 5.1 of Chapter I). With regard to an isolated quantum mechanical system with known particle composition and known particle potentials, let S be a closed sample space of order N and let $x_i^{(1)}$ $i = 1, \dots, N$, and $x_j^{(2)}$ $j = 1, \dots, N$ be different bases in S . Then

Fourth law of array assignment If mixed state of knowledge $Z^{(1)}$ in relation to basic property $x_i^{(1)}$ is recognisably *similar* to mixed state of knowledge $Z^{(2)}$ in relation to basic property $x_j^{(2)}$, we should set our density matrix $\rho_{kn}^{(1)}$ in the $x_i^{(1)}$ representation equal to our density matrix $\rho_{kn}^{(2)}$ in the $x_j^{(2)}$ representation.

We show in section 8 how the fourth law of array assignment can help in deriving the canonical distribution of quantum statistical mechanics.

8. Modelling of a thermodynamic system in equilibrium

The purpose of this section is to indicate how quantum statistical mechanics may be more clearly developed using our Bayesian interpretation of quantum mechanics. The advantages of a Bayesian approach to statistical mechanics have been constantly pointed out by Jaynes (see for example [28]). Many problematic concepts like ‘ergodic hypotheses’, ‘heat baths’ etc. can be avoided entirely. But with the more rigorous theory of mixed states made possible in the present interpretation of quantum mechanics the advantages of the Bayesian approach are even more apparent.

A real macroscopic system in thermal equilibrium (like a gas at a definite temperature in a closed container) may be modelled as an *isolated* quantum mechanical system of particles moving under known inter-particle potentials and external potentials.*

* In this way we avoid the need for a ‘heat bath’ (in thermal contact with the system) whose effect on the system is hard to take into account. We assume that errors arising from our having to guess the *exact* numbers of particles of the various kinds we take to be present are negligible. We will not here be

In particular the external potentials that constrain the particles to occupy a definite volume of space may be supposed known as well as any additional external fields to which the particles of the system may be subjected.

A system so modelled as a quantum mechanical system will have a Hamiltonian which may be time dependent (if the external conditions are changing). Whether the Hamiltonian is time dependent or not, there is a property of the system associated with the Hamiltonian called the energy E taking discrete values E_n generally a function of the time. This was explained in section 3 of Chapter XI. We identify the quantum mechanical energy E of the system with its classical thermodynamic internal energy, the only difference being that while the quantum mechanical energy has theoretically a definite value, the classical thermodynamic internal energy contains an arbitrary additive constant, or rather its zero point is chosen in a conventional way.

With regard to a system in thermodynamic equilibrium*, when we know the (constant) classical thermodynamic internal energy U to classical accuracy (as we may do in practice) we claim that we are then in a mixed state of knowledge regarding the quantum mechanical dynamical properties of the system involving effective knowledge of the expected energy \bar{E} of E given by

$$\bar{E} = U + U_0 \quad (8.1)$$

where U_0 is a constant that can always be identified at a later point. We now make the following fundamental claim of (equilibrium) quantum statistical mechanics.†

Claim regarding knowledge of the expected energy

Supposed knowledge of the expected value \bar{E} of the quantum mechanical energy E of the system amounts on its own to a mixed state of knowledge of the quantum mechanical system dynamics sufficient to account for all macroscopic thermodynamic properties of the system.

Therefore any additional information we may have about the classical thermodynamic properties (e.g. knowledge of the temperature or of the pressure (in the case of a gas)) is redundant.

So when we suppose our knowledge of the system dynamics consists only in the knowledge of the expected energy \bar{E} of the system, we are in a mixed state of knowledge. And by the law of orthogonal representation of mixed states of knowledge this can be represented by an array of N orthogonal wave functions where N is the dimension of any basis in the sample space of all propositions about all the quantum mechanical dynamical properties of the system. We write this array as

developing the grand canonical ensemble in which only the expected number of particles is taken as known (see p.10 of [28]).

* Any external conditions may still be subject to change, for example the known volume occupied by the system may be *gradually* changed while maintaining thermal equilibrium. We consider such (adiabatic) changes later on but for the present we assume the external conditions are fixed (and known).

† This will lead us to the canonical distribution.

$$\{\Phi(x_i|Y_1), \dots, \Phi(x_i|Y_N); w_1, \dots, w_N\} \quad (8.2)$$

and we seek suitable candidates for the orthogonal wave functions and the correct values for the weights.

8.1 Determination of a suitable set of orthonormal wave functions

Now in (8.2) we may take the x_i to refer to a basic *time-dependent* property at a time t during the time covered by our sample space (which can be as long as we please). Now consider the array

$$\{\Phi(x'_i|Y_1), \dots, \Phi(x'_i|Y_N); w_1, \dots, w_N\} \quad (8.1.1)$$

where the wave functions (for the same pure states of knowledge Y_1, \dots, Y_N) are over a basis x'_i that refers to the same property (as x_i) but at a later time t' during the time covered by our sample space. As noted in section 1, array (8.1.1) represents the same mixed state of knowledge of system dynamics as array (8.2), the weights being the same and the wave functions $\Phi(x_i|Y_j)$ in (8.2) and $\Phi(x'_i|Y_j)$ in (8.1.1) being related by Feynman's law, or equivalently, the wave functions $\Phi(x'_i|Y_j)$ being the time evolved forms of the $\Phi(x_i|Y_j)$ (as determined by the Schrödinger equation for the system). We cannot however immediately claim that the *density matrices* associated with arrays (8.2) and (8.1.1) are equal because the representations (based on x_i and on x'_i) are different.

But, because the system is in thermodynamic equilibrium our mixed state of knowledge in relation to the truth or falsity of any of the propositions x_i ($i=1, \dots, N$) referring to time t is evidently *similar* to our mixed state of knowledge regarding the truth or falsity of any of the propositions x'_i ($i=1, \dots, N$) referring to time t' . By the fourth law of array assignment the density matrix for array (8.2) must therefore equal that for array (8.1.1), or, put another way, the density matrix for array (8.2) must remain the same when the wave functions in it evolve according the Schrödinger equation while the weights remain constant. We can write the Schrödinger equation as

$$-\frac{\hbar}{i} \frac{\partial}{\partial t} \Phi(x_k|Y_j) = \sum_{k'} H_{kk'} \Phi(x_{k'}|Y_j) \quad (8.1.2)$$

the x_k referring to a general time t and the $N \times N$ matrix $H_{kk'}$ standing for the Hamiltonian. We know the Hamiltonian matrix is Hermitian, i.e. that it always satisfies

$$H_{kk'} = H_{k'k}^* \quad (8.1.3)$$

And in our modelling of the thermodynamic system we assume the particle potentials do not depend on the time explicitly, therefore $H_{kk'}$ is independent of t .

The density matrix going with our array (8.2) is

$$\rho_{kn} = \sum_j w_j \Phi(x_k|Y_j)\Phi^*(x_n|Y_j) \quad (8.1.4)$$

where the sum goes from $j=1$ to $j=N$ and as usual the limits are omitted for brevity.

Since ρ_{kn} must be independent of time, its partial derivative with respect to t must vanish. Differentiating (8.1.4) with respect to t remembering the weights are constant, we find by (8.1.2) that*

$$-\frac{\hbar}{i} \frac{\partial}{\partial t} \rho_{kn} = \sum_j w_j \left[\sum_{k'} \Phi^*(x_n|Y_j) H_{kk'} \Phi(x_{k'}|Y_j) - \sum_{n'} \Phi(x_k|Y_j) H_{nn'}^* \Phi^*(x_{n'}|Y_j) \right]. \quad (8.1.5)$$

Setting the RHS equal to zero, multiplying through by $\Phi(x_n|Y_{j'})\Phi^*(x_k|Y_{j'})$ and summing over n and k gives, on account of the orthogonality of the wave functions $\Phi(x_i|Y_j)$ for different values of j , the result

$$\sum_j w_j \left[\sum_{kk'} \delta_{jj'} \Phi^*(x_k|Y_{j'}) H_{kk'} \Phi(x_{k'}|Y_j) - \sum_{nn'} \delta_{jj'} \Phi(x_n|Y_{j'}) H_{nn'}^* \Phi^*(x_{n'}|Y_j) \right] = 0$$

or

$$w_{j'} \sum_{kk'} \Phi^*(x_k|Y_{j'}) H_{kk'} \Phi(x_{k'}|Y_{j'}) - w_{j''} \sum_{nn'} \Phi(x_n|Y_{j'}) H_{nn'}^* \Phi^*(x_{n'}|Y_{j''}) = 0.$$

But here the two sums are equal because of the Hermitian property (8.1.3) and so we obtain the requirement

$$(w_{j'} - w_{j''}) \sum_{kk'} \Phi^*(x_k|Y_{j''}) H_{kk'} \Phi(x_{k'}|Y_{j'}) = 0$$

or

$$(w_{j'} - w_{j''}) \sum_k \Phi^*(x_k|Y_{j''}) \sum_{k'} H_{kk'} \Phi(x_{k'}|Y_{j'}) = 0. \quad (8.1.6)$$

* This is the general law of evolution of the density matrix representing any mixed state of knowledge. It can evidently be written in the 'operator' form $(-\hbar/i)\partial\rho_{kn}/\partial t = \sum_{k'} H_{kk'}\rho_{k'n} - \sum_{n'} H_{nn'}^*\rho_{kn}$ which

bears a similarity to the Schrödinger equation (8.1.2) which of course is the general law of evolution of the wave function representing any pure state of knowledge.

The condition (8.1.6) means the function $\sum_{k'} H_{kk'} \Phi(x_{k'} | Y_{j'})$ of k must be orthogonal (in function space) to the function $\Phi(x_k | Y_{j''})$ whenever $w_{j'} \neq w_{j''}$.

So if all the weights have different values the function $\sum_{k'} H_{kk'} \Phi(x_{k'} | Y_{j'})$, i.e. the result of applying the Hamiltonian operator to any one of the functions $\Phi(x_k | Y_{j'})$, must be orthogonal to all the other functions $\Phi(x_k | Y_{j''})$ $j'' \neq j'$. Since the $\Phi(x_k | Y_j)$ form a complete orthogonal set $\sum_{k'} H_{kk'} \Phi(x_{k'} | Y_{j'})$ can therefore only be a constant times $\Phi(x_k | Y_{j'})$ itself, i.e. $\Phi(x_k | Y_{j'})$ can only be an eigenfunction of the Hamiltonian. Thus, when the weights are all different, the set of orthogonal functions in our density matrix are necessarily eigenfunctions of the Hamiltonian i.e. they must satisfy

$$\sum_{k'} H_{kk'} \Phi(x_{k'} | Y_{j'}) = E_{j'} \Phi(x_k | Y_{j'}), \quad (8.1.7)$$

where $E_{j'}$ is the corresponding eigenvalue of the Hamiltonian matrix.

If some of the weights are the same, condition (8.1.6) tells us only that the function $\sum_{k'} H_{kk'} \Phi(x_{k'} | Y_{j'})$ of k must be orthogonal to the functions $\Phi(x_k | Y_{j''})$ for which $w_{j''} \neq w_{j'}$. It must therefore lie in the subspace spanned by the functions $\Phi(x_k | Y_j)$ of the array for which the corresponding weights are equal to $w_{j'}$. Supposing just the first r weights are equal (and all the others unequal) we can therefore write

$$\sum_{k'} H_{kk'} \Phi(x_{k'} | Y_{j'}) = \sum_{j=1}^r A_{j'j} \Phi(x_k | Y_j), \quad j'' = 1, \dots, r \quad (8.1.8)$$

where the $A_{j'j}$ are complex constants. But the functions $\Phi(x_k | Y_j)$ in this subspace can be 'rotated together' in any way we please without changing the density matrix. That is we are free to make a unitary transformation to new wave functions $\Phi(x_k | \tilde{Y}_j)$ given by

$$\Phi(x_k | \tilde{Y}_j) = \sum_{j'} U_{jj'} \Phi(x_k | Y_{j'}), \quad (8.1.9)$$

where we now adopt the convention that j parameters are summed from 1 to r (while k parameters will still be summed from 1 to N). The transformation inverse to (8.1.9) is

$$\Phi(x_k | Y_{j''}) = \sum_j U_{j''j}^{-1} \Phi(x_k | \tilde{Y}_j), \quad j'' = 1, \dots, r. \quad (8.1.10)$$

With the new wave functions, the effect of the Hamiltonian operating on one can be written

$$\begin{aligned}\sum_{k'} H_{kk'} \Phi(x_{k'} | \tilde{Y}_{j''}) &= \sum_{k'} H_{kk'} \sum_j U_{j''j'} \Phi(x_{k'} | Y_{j'}) = \sum_j U_{j''j'} \sum_{k'} H_{kk'} \Phi(x_{k'} | Y_{j'}) \\ &= \sum_j U_{j''j'} \sum_{j'''} A_{jj'''} \Phi(x_k | Y_{j'''}) = \sum_{j'''} U_{j''j'} A_{jj'''} U_{j''j'''}^{-1} \Phi(x_k | \tilde{Y}_{j'''})\end{aligned}$$

So if we can choose our unitary transformation in a way that makes matrix $A_{jj'}$ diagonal we will have

$$\sum_{k'} H_{kk'} \Phi(x_{k'} | \tilde{Y}_{j''}) = \sum_{j'''} A_{j''} \delta_{j''j'''} \Phi(x_k | \tilde{Y}_{j'''}) = A_{j''} \Phi(x_k | \tilde{Y}_{j''}) \quad (8.1.11)$$

where $A_{j''}$ are the diagonal elements resulting from the diagonalisation of matrix $A_{jj'}$.

So if diagonalisation of matrix $A_{jj'}$ is possible we see that when the first r weights are equal, it is (by (8.1.11)) still the case that the wave functions of our representative array can be taken to be eigenfunctions of the Hamiltonian. And by similar arguments this can clearly be shown to be true also when any set of the weights are equal rather than the first r weights, and when there are several sets of equal weights. Relations of the kind (8.1.8) must hold for the wave functions associated with each set of equal weights, and unitary transformations could be applied to each to guarantee they were eigenfunctions of the Hamiltonian.

It remains only to show that the matrix $A_{jj'}$ can always be diagonalised by means of a unitary transformation. Starting with (8.1.8) as representative of the general case of an equal set of weights, we multiply through by $\Phi^*(x_k | Y_{j''})$ and sum over k :

$$\sum_{kk'} \Phi^*(x_k | Y_{j''}) H_{kk'} \Phi(x_{k'} | Y_{j''}) = \sum_{kj} \Phi^*(x_k | Y_{j''}) A_{j''j} \Phi(x_k | Y_j).$$

Orthonormality of the $\Phi(x_k | Y_j)$ makes the RHS equal to $A_{j''j''}$ so we find

$$A_{j''j''} = \sum_{kk'} \Phi^*(x_k | Y_{j''}) H_{kk'} \Phi(x_{k'} | Y_{j''})$$

and since the Hamiltonian matrix is Hermitian this shows that matrix $A_{j''j''}$ is also Hermitian, i.e. that

$$A_{j''j''}^* = A_{j''j''} \quad j'', j''' = 1, \dots, r$$

and therefore can always be diagonalised by a unitary transformation.

We have thus found suitable candidates for the orthogonal wave functions of our representative array (8.2). They can be taken to be a complete set of N orthonormal eigenfunctions of the system's quantum mechanical (time independent) Hamiltonian. Next we must find the values of the corresponding weights.

8.2 Determination of the weights in the representative array

Taking up the notation in section 3 of Chapter XI, the orthonormal (time independent) eigenfunctions of the system Hamiltonian are written as $\phi_{nl}(q)$ where q stands for the coordinates of the system (i.e. the particle position coordinates and the z components of particle spins relative to a fixed Cartesian coordinate system), parameter n quantifies the energy E_n of the system and parameter l quantifies the other properties of the system associated with the complete set of orthogonal wave functions $\phi_{nl}(q)e^{-iE_n t/\hbar}$ (see section 3 of Chapter XI). Since the present system occupies a finite volume of space the possible energies form a discrete set of values so we may take n to have integer values with E_n increasing monotonically with n . The parameter l also has discrete values but generally stands for a *number* of discrete parameters. The possible values of l are generally dependent on the value of n (as we saw, for example, in section 3.1.2 of Chapter XI).

To represent our mixed state of knowledge of the quantum mechanical system (used to model the macroscopic thermodynamic system in equilibrium) we adopt the array

$$\{\phi_{nl}(q); w_{nl}\} \quad (8.2.1)$$

where $\phi_{nl}(q)$ stands for the set of functions $\phi_{nl}(q)$ for all possible values of n and l , and w_{nl} stands for the set of corresponding weights. The array (8.2.1) will serve for all times during which our system is in thermodynamic equilibrium. The time factor $e^{-iE_n t/\hbar}$ need not be included in the wave functions of array (8.2.1) because it does not alter the density matrix

$$\rho_{qq'} = \sum_{nl} w_{nl} \phi_{nl}(q) \phi_{nl}^*(q') \quad (8.2.2)$$

where the summation is over all values of l for given n and then for all values of n .^{*} Any phase factor $e^{i\beta_{nl}}$ that may attend the wave functions also does not affect the density

^{*} Strictly speaking we should write any sum of the kind $\sum_{nl} S_{nl}$ as $\sum_n \left(\sum_l S_{nl} \right)$ because the possible

values of l are dependent on the value of n and the order of the summations is not reversible. We refrain from doing this only in the interests of simplification.

matrix. So the absolute phases of the eigenfunctions $\phi_{nl}(q)$ can be chosen in any way. The number of possible values of n is infinite (the number of parameters l being finite for each value of n). In any particular case we will need to show that the summation in (8.2.2) converges to a finite value for all q and q' .

In terms of the array (8.2.1) the expected value \bar{E} of the system energy is, by (2.1.4),

$$\bar{E} = \sum_{nl} w_{nl} E_n \quad (8.2.3)$$

with standard deviation

$$\sigma_E = \sqrt{\sum_{nl} w_{nl} (E_n - \bar{E})^2}. \quad (8.2.4)$$

To find the values of the weights w_{nl} we apply the method of maximum information entropy (section 5). Accordingly the w_{nl} are the values that maximise

$$S = -\sum_{nl} w_{nl} \ln w_{nl} \quad (8.2.5)$$

subject to the constraints

$$\bar{E} = \sum_{nl} w_{nl} E_n \quad \text{and} \quad \sum_{nl} w_{nl} = 1. \quad (8.2.6)$$

in which \bar{E} is supposed known. Using Lagrange's method we maximise

$$-\sum_{nl} w_{nl} \ln w_{nl} + \mu \sum_{nl} w_{nl} E_n + \lambda \sum_{nl} w_{nl} \quad (8.2.7)$$

subject to no constraints then apply (8.2.6) to determine the parameters μ and λ . Setting to zero the change in (8.2.7) under a variation δw_{nl} in w_{nl} we get

$$-\sum_{nl} (\delta w_{nl} \ln w_{nl} + w_{nl} \frac{1}{w_{nl}} \delta w_{nl}) + \mu \sum_{nl} \delta w_{nl} E_n + \lambda \sum_{nl} \delta w_{nl} = 0$$

or

$$\sum_{nl} (\ln w_{nl} + 1 - \mu E_n - \lambda) \delta w_{nl} = 0.$$

Since this must hold for all small variations we must have

$$\ln w_{nl} + 1 - \mu E_n - \lambda = 0$$

or replacing $1 - \lambda$ by λ and $-\mu$ by μ (i.e. by redefining the parameters) we have, for the required weights in our representative array, the expression

$$w_{nl} = e^{-\lambda - \mu E_n} \quad (8.2.8)$$

with formulae

$$\left. \begin{aligned} \sum_{nl} e^{-\mu E_n} &= e^\lambda \\ \sum_{nl} e^{-\lambda - \mu E_n} E_n &= \bar{E} \end{aligned} \right\} \quad (8.2.9)$$

for the parameters μ and λ in (8.2.8).

A proof that (8.2.9) has only one solution for μ and λ , and that this solution *maximises* S in (8.2.5) rather than minimising it, is given in Appendix E.

We note that the required weights, as given by (8.2.8) conform to the well known canonical distribution in the usual theory of statistical mechanics.

It remains only to identify the parameters μ and λ .

8.3 Identification of μ and λ with certain thermodynamic properties

Note that in (8.2.9) we have

$$\sum_{nl} e^{-\mu E_n} = \sum_n \left(\sum_l e^{-\mu E_n} \right) = \sum_n e^{-\mu E_n} L_n \quad (8.3.1)$$

where

$$L_n = \sum_l 1 \quad (8.3.2)$$

(i.e. 1 added to itself as many times as there are l values for given n) is the degeneracy of the energy level E_n .

By (8.2.9) the quantity λ is given by

$$\lambda = \ln \sum_{nl} e^{-\mu E_n} \quad (8.3.3)$$

and we identify this and μ with macroscopic thermodynamic properties as follows.

As λ is by (8.3.3) a function of μ and the E_n we will have formally, for any infinitesimal variations the relation

$$d\lambda = \frac{\partial\lambda}{\partial\mu} d\mu + \sum_n \frac{\partial\lambda}{\partial E_n} dE_n \quad (8.3.4)$$

where, by (8.3.3)

$$\frac{\partial\lambda}{\partial\mu} = \frac{\sum_{nl} (-E_n) e^{-\mu E_n}}{\sum_{nl} e^{-\mu E_n}} = -\bar{E}$$

the last step being a consequence of (8.2.9). Also, by (8.3.3)

$$\frac{\partial\lambda}{\partial E_n} = \frac{\sum_{ml} (-\mu) e^{-\mu E_m} \delta_{nm}}{\sum_{ml} e^{-\mu E_m}}$$

where by (8.2)

$$\sum_{ml} e^{-\mu E_m} \delta_{nm} = \sum_m \left(\sum_l e^{-\mu E_m} \delta_{nm} \right) = \sum_l e^{-\mu E_n} = e^{-\mu E_n} L_n$$

Hence

$$\frac{\partial\lambda}{\partial E_n} = -\mu \frac{e^{-\mu E_n} L_n}{\sum_{ml} e^{-\mu E_m}} = -\mu e^{-\lambda - \mu E_n} L_n$$

and in (8.3.4)

$$\sum_n \frac{\partial\lambda}{\partial E_n} dE_n = \sum_n -\mu e^{-\lambda - \mu E_n} L_n dE_n = -\mu \sum_{nl} e^{-\lambda - \mu E_n} dE_n$$

so using (8.2.8), (8.3.4) becomes

$$d\lambda = -\bar{E} d\mu - \mu \sum_{nl} w_{nl} dE_n \quad (8.3.5)$$

where by the second of (8.2.9) we have

$$\bar{E} = \sum_{nl} w_{nl} E_n \quad (8.3.6)$$

If we start (say at time t_1) making known reversible adiabatic variations in the external conditions (i.e. making slow changes to the external fields) this in no way changes our mixed state of knowledge in relation to times $t < t_1$ when the external fields are fixed. This is because knowledge of future external fields is redundant. Therefore assuming only that our knowledge remains mixed, the array $\{\phi_{nl}(q); w_{nl}\}$ (with the same weights) serves just as well to represent our knowledge in relation to times $t \geq t_1$ so long as the functions $\phi_{nl}(q)$ are (for each n and l) now changing appropriately with time. The continuity of representation by array $\{\phi_{nl}(q); w_{nl}\}$ is guaranteed by the *law of natural evolution of an array* claimed in section 1 because the $\phi_{nl}(q)$ (or rather their correct forms as on the RHS of (4.19) of Chapter XI which differ in a way unimportant as far as the density matrix and therefore the representation by $\{\phi_{nl}(q); w_{nl}\}$ is concerned) satisfy the Schrödinger equation under the changing external fields.

Since the w_{nl} remain constant during reversible adiabatic variations, for any small (quasi-static) variations of that kind (8.3.6) gives

$$d\bar{E} = \sum_{nl} w_{nl} dE_n \quad (8.3.7)$$

and (8.3.5) gives $d\lambda = -\bar{E}d\mu - \mu d\bar{E}$ or

$$d(\lambda + \mu\bar{E}) = 0. \quad (8.3.8)$$

So the quantity $\lambda + \mu\bar{E}$ remains constant under any reversible adiabatic variation. This leads us to identify $\lambda + \mu\bar{E}$ with the thermodynamic entropy S of the system, because the entropy is the thermodynamic property that stays constant under reversible adiabatic changes. Actually any function of the entropy will also stay constant and we should identify $\lambda + \mu\bar{E}$ as some function $\chi(S)$ of S but of S alone.

The form of the function $\chi(S)$ can be found (as in p.13 of [27]) by considering two separate thermodynamic systems A and B at the same temperature. Modelling both as quantum mechanical systems with expected energies \bar{E}_A and \bar{E}_B assumed known, we are in a mixed state of knowledge with regard to each. Formulae (8.2.8) and (8.2.9) will apply to each with λ written as λ_A and λ_B , and μ written as μ_A and μ_B accordingly, and we can identify $\lambda_A + \mu_A\bar{E}_A$ and $\lambda_B + \mu_B\bar{E}_B$ as functions $\chi_A(S_A)$ and $\chi_B(S_B)$ of the thermodynamic entropies S_A and S_B of systems A and B respectively.

But we are also at liberty to regard systems A and B as together forming a single system at a uniform temperature and to apply the same theory to it. We take all the equations and terms in section 8.2 to refer to that system. Now assuming (as it seems we may) that the sample spaces referring to systems A and B are *logically independent* under all our knowledge, the stationary state wave functions $\phi_{nl}(q)$ will be the products $\phi_{n_A l_A}(q_A) \cdot \phi_{n_B l_B}(q_B)$ of those for each component system and the corresponding weights

w_{nl} will be the products $w_{n_A l_A} \cdot w_{n_B l_B}$ of the weights of each component system (see section 3).

It is useful for the present purpose to relax our notation according to which, in for example $\phi_{nl}(q)$, n is a single parameter quantifying the corresponding energy E_n . Instead we allow parameters nl to label (uniquely) the wave functions $\phi_{nl}(q)$ in *any* way with the corresponding energy values denoted E_{nl} some of which may be the same. So letting nl stand for $n_A l_A n_B l_B$ and we will have

$$E_{nl} = E_{n_A l_A} + E_{n_B l_B}.$$

Therefore, by (8.2.8)

$$w_{nl} = e^{-\lambda - \mu(E_{n_A l_A} + E_{n_B l_B})}$$

and since

$$w_{nl} = w_{n_A l_A} \cdot w_{n_B l_B}$$

the formula (8.2.8) applied to systems A and B on their own gives

$$w_{nl} = e^{-\lambda - \mu(E_{n_A l_A} + E_{n_B l_B})} = e^{-(\lambda_A + \lambda_B) - \mu_A E_{n_A l_A} - \mu_B E_{n_B l_B}}$$

for all $n_A l_A$ and all $n_B l_B$ independently.* This can only mean that

$$\left. \begin{aligned} \mu &= \mu_A = \mu_B \\ \lambda &= \lambda_A + \lambda_B \end{aligned} \right\} \quad (8.3.9)$$

Therefore for all systems at the same temperature, μ has the same value. That is μ is a function of the temperature only. And λ is an additive property for systems at one and the same temperature. It follows that $\lambda + \mu \bar{E}$ is also additive and since the thermodynamic entropy S is additive in the same sense we must have

$$\chi_A(S_A) + \chi_B(S_B) = \chi_{AB}(S_A + S_B)$$

* Note also that by substituting $w_{nl} = w_{n_A l_A} \cdot w_{n_B l_B}$ in (8.2.3) in which E_n is now $E_{nl} (= E_{n_A l_A} + E_{n_B l_B})$ and nl stands for $n_A l_A n_B l_B$ we easily show that $\bar{E} = \bar{E}_A + \bar{E}_B$. That is, the expected energy is an additive property for systems at one and the same temperature.

where χ_{AB} is $\lambda + \mu\bar{E}$ written as a function of the entropy S of the combined system. Since S_A and S_B are independently variables, differentiating this equation with respect to S_A and with respect to S_B we find

$$\chi'_A(S_A) = \chi'_B(S_B) = \chi'_{AB}(S_A + S_B)$$

showing that $\chi'(S)$ can only be a universal constant say $1/k$. So $\chi(S) = S/k$ and for any thermodynamic system modelled quantum mechanically

$$\lambda + \mu\bar{E} = \frac{1}{k} S \quad (8.3.10)$$

By inserting (8.2.8) into (8.2.5) and applying (8.3.6) we see that $\lambda + \mu\bar{E}$ equals the information entropy, i.e. the degree of our ignorance of system dynamics given we know only the expected energy. (That is, the degree of our ignorance over-and-above our unavoidable ignorance due to the uncertainty principle.) Hence (8.3.10) gives a relation between the thermodynamic entropy of an isolated system and our information entropy. The first is just k times the second.

Now under slow (reversible) injection of heat into the system with external conditions held constant (e.g. with the volume occupied by a gas held constant) we have the thermodynamic relation $dU = TdS + dW$ in which T is the absolute temperature (in $^\circ K$) and the work done is zero, i.e. $dW = 0$. Identifying the change dU in internal energy with $d\bar{E}$ we therefore expect

$$\frac{\partial S}{\partial \bar{E}} = \frac{1}{T}.$$

where the partial derivative refers to constant external conditions (constant volume in the case of a gas). Applying this to (8.3.10) we find

$$\frac{\partial \lambda}{\partial \mu} \frac{\partial \mu}{\partial \bar{E}} + \frac{\partial \mu}{\partial \bar{E}} \bar{E} + \mu = \frac{1}{kT}. \quad (8.3.11)$$

Since external conditions are fixed the wave functions $\phi_{nl}(q)$ in our representative array $\{\phi_{nl}(q); w_{nl}\}$ together with the associated energy eigenvalues E_n remain constant (only the weights w_{nl} change). Hence

$$\frac{\partial \lambda}{\partial \mu} = \frac{\partial}{\partial \mu} \ln \sum_{nl} e^{-\mu E_n} = \frac{\sum_{nl} (-E_n) e^{-\mu E_n}}{\sum_{nl} e^{-\mu E_n}}$$

which by (8.2.9) is just $-\bar{E}$. So (8.3.11) gives

$$\mu = \frac{1}{kT} \quad (8.3.12)$$

and by (8.3.10)

$$k\lambda = S - \frac{1}{T} \bar{E} \quad (8.3.13)$$

which relates λ to the thermodynamic entropy, the absolute temperature and the expected energy of the system. The latter we have identified with the internal energy as in relation (8.1). This identification is only specified to within an additive constant (U_0 in (8.1)) so λ too is identified only to within a (related) additive constant.*

8.4 The value of the constant k and the case of the perfect gas

For the purpose of finding the value of k and of illustrating the derivation of equations of state, we consider the simple case of the perfect gas, or more precisely the case of many non-interacting spin-less (non-identical) particles of the same mass enclosed in a box. We need consider only the case in which external conditions may be changed by adjusting the length a of one side of the box.

With coordinates chosen as in section 3.1.1 of Chapter XI the wave functions $\phi_{n_l}(q)$ in our representative array $\{\phi_{n_l}(q); w_{n_l}\}$ are products of the wave functions

$$\phi_{n_1 n_2 n_3}(x, y, z) = \sqrt{\frac{8}{abc}} \sin \frac{n_1 \pi x}{a} \sin \frac{n_2 \pi y}{b} \sin \frac{n_3 \pi z}{c} \quad (8.4.1)$$

in (3.1.1.1) of Chapter XI, for all N particles present. The energy associated with (8.4.1) is, by (3.1.1.3) of Chapter XI

$$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right). \quad (8.4.2)$$

* It is not the case that by (8.3.13) \bar{E} is necessarily zero at absolute zero because as $T \rightarrow 0$ we have by (8.3.12) that $\mu \rightarrow \infty$ and therefore (by (8.2.9)) $\lambda \rightarrow -\infty$. In multiplying (8.3.13) through by T and letting $T \rightarrow 0$ it is then not necessarily the case that $T\lambda \rightarrow 0$.

In our array $\{\phi_{nl}(q); w_{nl}\}$ we now replace the parameters nl by the parameters $n_1^{(1)}n_2^{(1)}n_3^{(1)}\dots n_1^{(N)}n_2^{(N)}n_3^{(N)}$ i.e. for the combined triplets $n_1n_2n_3$ for each particle, each n taking values $1,2,\dots,\infty$.^{*} And the energy going with the stationary wave function $\phi_{nl}(q)$ is

$$E_{n_1^{(1)}n_2^{(1)}n_3^{(1)}} + \dots + E_{n_1^{(N)}n_2^{(N)}n_3^{(N)}} = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^{(1)2} + \dots + n_1^{(N)2}}{a^2} + \frac{n_2^{(1)2} + \dots + n_2^{(N)2}}{b^2} + \frac{n_3^{(1)2} + \dots + n_3^{(N)2}}{c^2} \right) \dots(8.4.3)$$

We thus have for the value of e^λ in (8.2.9) the expression

$$e^\lambda = \sum_{n_1^{(1)}n_2^{(1)}n_3^{(1)}\dots n_1^{(N)}n_2^{(N)}n_3^{(N)}} e^{-\mu(E_{n_1^{(1)}n_2^{(1)}n_3^{(1)}} + \dots + E_{n_1^{(N)}n_2^{(N)}n_3^{(N)}})} \quad (8.4.4)$$

Substitution of (8.4.3) into this gives a product of sums of the form

$$\sum_{n=1}^{\infty} e^{-\alpha n^2}$$

with different (positive) values of α independent of n . The values of α are in practice usually exceedingly small compared to 1 enabling us to use the approximation

$$\sum_{n=1}^{\infty} e^{-\alpha n^2} = \int_0^{\infty} e^{-\alpha u^2} du + O(1)$$

where the error is (as indicated) of order 1. The integral has the analytical value $\sqrt{\pi}/(2\sqrt{\alpha})$ so the condition for replacing the sum by the integral is that[†]

$$\frac{\sqrt{\pi}}{2\sqrt{\alpha}} \gg 1.$$

Using the integral approximation (8.4.4) becomes

$$e^\lambda = \left(\frac{1}{2} \sqrt{\frac{\pi}{\mu \frac{\pi^2 \hbar^2}{2ma^2}}} \right)^N \left(\frac{1}{2} \sqrt{\frac{\pi}{\mu \frac{\pi^2 \hbar^2}{2mb^2}}} \right)^N \left(\frac{1}{2} \sqrt{\frac{\pi}{\mu \frac{\pi^2 \hbar^2}{2mc^2}}} \right)^N = \left(\frac{1}{2\hbar} \sqrt{\frac{2m}{\pi\mu}} \right)^{3N} V^N$$

^{*} To maintain the original parameters nl would be again to create quite unnecessary difficulties. It is often sufficient to remember that any sum over parameters nl is a sum over all the possible stationary state labels.

[†] In the modelling of gases α is, as can be verified later, generally of the order of 10^{-16} (see for example p. 41 of Rushbrooke [29]) and this condition is well satisfied.

where $V (= abc)$ is the internal volume of the box. Hence

$$\lambda = \ln \sum_n e^{-\mu E_n} = N \ln V + 3N \ln \left(\frac{1}{2h} \sqrt{\frac{2m}{\pi\mu}} \right) \quad (8.4.5)$$

From the thermodynamic relation $dU = TdS - pdV$ and the relation

$$kd\lambda = dS - \frac{1}{T} d\bar{E}$$

derived from (8.3.13) assuming a constant temperature, we obtain, on identifying $d\bar{E}$ with dU , the result

$$p = Tk \left. \frac{\partial \lambda}{\partial V} \right|_T$$

giving by (8.4.5) the equation of state

$$pV = NkT. \quad (8.4.6)$$

Comparing (8.4.6) with the well known (classical thermodynamics) equation of state for a perfect gas in the form

$$pV = nRT$$

where n is the number of moles of gas present and $R = 8.315 \text{ J/}^\circ\text{K}$ is the universal gas constant we obtain for k the value

$$k = \frac{nRT}{NT} = \frac{R}{N_A}$$

where $N_A (= N/n)$ is Avogadro's number (the number of molecules per mole) equal to 6.022×10^{23} . This gives for k (which is of course Boltzman's constant) the value $k = 1.380 \times 10^{-23} \text{ J/}^\circ\text{K}$.

Finally we derive the formula for the internal energy \bar{E} . By (8.2.9), since the possible energy levels of the system remain the same when the volume is fixed (meaning the dimensions of the box are kept the same), we can write

$$\bar{E} = - \frac{\left(\frac{\partial}{\partial \mu} e^\lambda \right)_V}{e^\lambda} = - \left(\frac{\partial \lambda}{\partial \mu} \right)_V.$$

Using (8.4.5) for λ , we therefore obtain

$$\bar{E} = \frac{3}{2} N \frac{1}{\mu} = \frac{3}{2} NkT \quad (8.4.7)$$

for the internal energy of the gas. If we define the classical thermodynamic internal energy U of a perfect gas (i.e. choose its additive constant) to be such that U vanishes at absolute zero then \bar{E} and U coincide exactly.

Differentiating (8.4.7) with respect to T keeping the volume constant gives the specific heat at constant volume as

$$C_v = \left. \frac{\partial \bar{E}}{\partial T} \right|_v = \frac{3}{2} Nk. \quad (8.4.8)$$

8.5 The likely deviation of the system energy from its expected value

When we suppose knowledge of the expected energy \bar{E} of the system (viewed as a quantum mechanical system) we claim (as we have said) to be in a mixed state of knowledge regarding system dynamics and on that basis we have deduced the form of an array $\{\phi_{nl}(q); w_{nl}\}$ representing that state of knowledge. As explained in section 2 we are therefore in a position to calculate our *degree of belief* distribution over the property values nl . This degree of belief distribution is none other than the function w_{nl} of nl which is calculated to be as given in (8.2.8) in which λ and μ are given by (8.2.9). This distribution will (by summing over l) give us also our degree of belief distribution over the possible energy levels E_n of the system. And with regard to that distribution its mean value (given by the first of (8.2.6)) is of course known already.

But of interest also is the standard deviation σ_E (defined in (8.2.4)) of the actual energy from its expected value. An expression for this in terms of thermodynamic properties can now be obtained assuming the validity of the identification of \bar{E} with the internal energy and of λ and μ with other thermodynamic properties as explained.

Expanding the bracket in (8.2.4) we find

$$\sigma_E^2 = \sum_{nl} w_{nl} (E_n - \bar{E})^2 = \sum_{nl} (w_{nl} E_n^2 - 2E_n \bar{E} w_{nl} + w_{nl} \bar{E}^2) \quad (8.5.1)$$

where the last term in the summand gives simply \bar{E}^2 and the second term in the summand gives $-2\bar{E}^2$. To evaluate what the first term in the summand gives we start again with the equality

$$\bar{E} = \frac{\sum_{nl} E_n e^{-\mu E_n}}{\sum_{nl} e^{-\mu E_n}}$$

which comes from (8.2.9) and differentiate it with respect to μ keeping the external conditions (and therefore the E_n values) constant. This provides the equation

$$\frac{\partial \bar{E}}{\partial \mu} = -\frac{\sum_{nl} E_n^2 e^{-\mu E_n}}{\sum_{nl} e^{-\mu E_n}} + \frac{\left(\sum_{nl} E_n e^{-\mu E_n} \right)^2}{\left(\sum_{nl} e^{-\mu E_n} \right)^2}.$$

Here the last term is \bar{E}^2 so the equation gives

$$\sum_{nl} w_{nl} E_n^2 = -\frac{\partial \bar{E}}{\partial \mu} + \bar{E}^2.$$

Substituting this in (8.5.1) we find

$$\sigma_E^2 = \sum_{nl} w_{nl} (E_n - \bar{E})^2 = -\frac{\partial \bar{E}}{\partial \mu}.$$

Since μ is simply related to the temperature by (8.3.12) we have

$$\frac{\partial \bar{E}}{\partial \mu} = \frac{\partial \bar{E}}{\partial T} \frac{\partial T}{\partial \mu} = -\frac{\partial \bar{E}}{\partial T} kT^2$$

so we have

$$\sigma_E^2 = kT^2 C$$

where

$$C = \frac{\partial \bar{E}}{\partial \mu}$$

is the specific heat of the system under constant external conditions, i.e. without external work. The ratio of the standard deviation to the expected energy itself can therefore be expressed as

$$\frac{\sigma_E}{\bar{E}} = \frac{T}{\bar{E}} \sqrt{kC} \quad (8.5.2)$$

and for consistency of the whole theory we require this to be exceedingly small compared to 1.

In the case of the perfect gas, we have (8.4.7) for \bar{E} and (8.4.8) for the specific heat at constant volume. With these values we find from (8.5.2) that

$$\frac{\sigma_E}{\bar{E}} = \frac{T}{\frac{3}{2}NkT} \sqrt{k \frac{3}{2}Nk} = \frac{1}{\sqrt{\frac{3}{2}N}}. \quad (8.5.3)$$

As N is generally of the order of Avogadro's number 6.022×10^{23} the requirement for σ_E/\bar{E} to be small is fulfilled well enough. In fact the whole distribution over the possible energy values is highly concentrated near to \bar{E} .

At first sight it is unclear from the simple exponential form of the distribution w_{nl} in (8.2.8) how our degree of belief distribution over energy values can be so sharp (so concentrated around \bar{E}). The reason is that the number of stationary quantum states whose energies lie in a classically small range E to $E + \Delta E$ grows rapidly with E . For example, in the case of the modelling of a perfect gas in section 8.4, the stationary quantum states are represented by points in a discrete $3N$ dimensional space corresponding to (natural number) coordinates $n_1^{(1)}, n_2^{(1)}, n_3^{(1)}, \dots, n_1^{(N)}, n_2^{(N)}, n_3^{(N)}$ and if the sides a, b and c of the box are equal, the energy of the stationary states is proportional to the square of the distance r from the origin of the $3N$ dimensional space. The number of stationary states for which r lies between r and $r + \Delta r$ (where Δr represents a classically small energy spacing) is proportional to the volume of space between the hyperspheres of radii r and $r + \Delta r$ or to the surface area of the hypersphere radius r times the distance Δr , i.e. proportional to $r^{3N-1} \Delta r$. By (8.2.8) the weight to be attached to stationary states in this 'spherical shell' is therefore proportional to $r^{3N-1} e^{-\alpha r^2} \Delta r$ where α is a positive constant. And since E is proportional to r^2 our degree of belief distribution over E is proportional to $E^{\frac{3}{2}N-1} e^{-\beta E}$ where β is positive constant. So $2\beta E$ follows a chi-square distribution with $3N$ degrees of freedom, its mean value being $3N$ and its standard deviation $\sqrt{6N}$. Since N is so very large, this chi-square distribution is essentially a normal distribution so the whole distribution is concentrated very close to its mean value, i.e. there is no significant part of it (or no significant tail extending out) far from the mean value.

9. Harmless conditioning under mixed states of knowledge

The possibility of harmless conditioning generalises to the case of mixed states. Having obtained mixed knowledge Z of a system S referred to sample space S covering a time period t_0 to t_1 , we claim we can, by observation learn by chance at time t_2 (where

$t_0 < t_2 < t_1$) the truth of a disjunction A of propositions x_i of any *primary* basis x of S referring to time t_2 . This can be achieved instantly and harmlessly with respect to the properties claimed by the propositions of the basis x (but not of course harmlessly with respect to other bases in S).

From time t_2 we are then in a mixed state of knowledge AZ in relation to S' which includes only the propositions of S that relate to times t_2 to t_1 . If our original state of knowledge Z is represented by array (1.1), where we suppose x_i is a *primary* basis, then our mixed state of knowledge AZ will be represented by the array

$$\{\Phi(x_i|AY_1), \dots, \Phi(x_i|AY_m); w_1, \dots, w_m\} \quad (9.1)$$

where the weights remain the same and the wave functions are those that would apply after the same harmless conditioning under the pure states of knowledge Y_j ($j = 1, \dots, m$). Those wave functions take the form calculated for them in section 4 of Chapter II, i.e.

$$\Phi(x_i|AY_j) = \begin{cases} \frac{\Phi(x_i|Y_j)}{\Phi(A|Y_j)} e^{-ik_j} & x_i \in A \\ 0 & x_i \notin A \end{cases} \quad (9.2)$$

where k_j is the (indeterminate) phase characteristic of knowledge Y_j .

10. Quasi-classical mixed states of knowledge

In addition to quasi-classical *pure* states of knowledge of a quantum mechanical process, under which we expect that over a time period the particles in question move approximately in a classical manner and more and more precisely so in a certain limit (see leading paragraphs in Chapter XII), there are quasi-classical *mixed* states of knowledge where the same applies. The correspondence principle in section 3.4 of Chapter III holds true for quasi-classical mixed states as well as for quasi-classical pure states.

The general quasi-classical mixed state of knowledge is represented by an array of the form (1.1) in which the wave functions, formally represented by $\Phi(x_i|Y_j)$ ($j = 1, \dots, m$), are all quasi-classical over the time period. During that time period we claim that (to classical accuracy) the n particles of the system follow classical paths under the system potential or the representative point in the $3n$ dimensional particle position configuration space follows a classical path in that space which is one of the possible classical paths associated with one of the wave functions $\Phi(x_i|Y_j)$. And the degree of belief we should assign to such a path is the degree of belief we would apply if we were in the quasi-

classical pure state of knowledge (represented by $\Phi(x_i|Y_j)$) times the corresponding weight w_j in our array.

This rule for the degree of belief in the classical orbits assumes that the classical orbits represented by the $\Phi(x_i|Y_j)$ ($j=1,\dots,m$) are different (each orbit unique to one wave function). If this is not the case some of the degrees of belief will have to be compounded (added) to give the net degree of belief to assign to a particular orbit.

In any case when the degree of belief of each orbit is calculated, the degree of belief density at any point and any time in $3n$ dimensional particle (position) configuration space can be calculated as can the degree of belief density in $3n$ dimensional particle momentum space, or in the $6n$ dimensional particle position/momentum space. In particular, we see the possibility, when working to classical accuracy, of holding a joint probability distribution over position r and momentum p of a single particle when our knowledge of the dynamical properties of the particle is of a certain kind.

11. Part-quasi-classical mixed states

As well as quasi-classical mixed states of knowledge of a quantum mechanical system over time there are part-quasi-classical mixed states of knowledge. These generalise the part-quasi-classical pure states of knowledge in section 1.4 of Chapter XII.

A part-quasi-classical mixed state of knowledge of the orbital motion of a system of n particles over a time period is represented by an array $\{\Phi(x_i|Y_1),\dots,\Phi(x_i|Y_m); w_1,\dots,w_m\}$ (of the form (1.1)) in which each wave function $\Phi(x_i|Y_j)$ ($j=1,\dots,m$) is a part-quasi-classical wave function, i.e. one which may be expressed thus:

$$\Phi(x_i|Y_j) = k_j^{(0)}\Phi_0(x_i|Y_j) + k_j^{(qc)}\Phi_{qc}(x_i|Y_j) \quad (11.1)$$

(cf. (1.4.1) of Chapter XII) where we take the basis x_i to represent the coordinates of all the n particles of the system in configuration space. The (normalised) quasi-classical part $\Phi_{qc}(x_i|Y_j)$ is (for any j) well separated (in configuration space) from the non-quasi-classical part $\Phi_0(x_i|Y_j)$ (which is also normalised).

We claim that under the part-quasi-classical mixed state of knowledge and during the time period in question, either the particles are moving (to classical accuracy) in a classical manner as they would under the mixed state of knowledge

$$\{\Phi_{qc}(x_i|Y_1),\dots,\Phi_{qc}(x_i|Y_m); l_1 w_1,\dots,l_m w_m\} \quad (11.2)$$

or the particles are occupying regions of space as they would under the mixed state of knowledge

$$\{\Phi_0(x_i|Y_1), \dots, \Phi_0(x_i|Y_m); p_1 w_1, \dots, p_m w_m\} \quad (11.3)$$

the factors l_j in (11.2) and p_j in (11.3) being given by

$$l_j = \frac{|k_j^{(qc)}|^2}{\sum_{j'=1}^m |k_{j'}^{(qc)}|^2 w_{j'}}, \quad \text{and} \quad p_j = \frac{|k_j^{(0)}|^2}{\sum_{j'=1}^m |k_{j'}^{(0)}|^2 w_{j'}}. \quad (11.4)$$

And the probabilities for one or other possibility are

$$\phi_{qc} = \sqrt{\sum_{j'=1}^m |k_{j'}^{(qc)}|^2 w_{j'}} e^{i\alpha}, \quad \text{and} \quad \phi_0 = \sqrt{\sum_{j'=1}^m |k_{j'}^{(0)}|^2 w_{j'}} e^{i\beta} \quad (11.5)$$

respectively, α and β being indeterminate phases. Since (for each j)

$$|k_j^{(qc)}|^2 + |k_j^{(0)}|^2 = 1 \quad (11.6)$$

in (11.1), we have by (11.5) and (1.2) that (as required)

$$|\phi_{qc}|^2 + |\phi_0|^2 = 1. \quad (11.7)$$

The above law of part-quasi-classical mixed states is meant to include cases in which some of the $k_j^{(qc)}$ or the $k_j^{(0)}$ are zero, i.e. to cases where some of the wave functions of the array representing our part-quasi-classical mixed state of knowledge are simply ordinary wave functions *or* simply quasi-classical wave functions (not superpositions of these types). Then (11.1)-(11.7) still formally apply and some of the weights in arrays (11.2) and (11.3) are zero and their corresponding wave functions may be set equal to any wave functions we choose (see the penultimate paragraph of section 1).

In particular if all the $\Phi(x_i|Y_j)$ ($j = 1, \dots, m$) are quasi-classical except for one (say the wave functions corresponding to $j = 1$) then all the weights in (11.3) are zero except for the first (which is equal to 1) while just the first weight in (11.2) is zero. Since arrays, some of whose weights are zero, can be reduced by leaving out those weights and their corresponding wave functions, it follows that in this case (11.3) is an array representing the pure state of knowledge $\Phi_0(x_i|Y_1)$.

Note that we are not generally claiming that we should be either in the mixed state of knowledge represented by array (11.2) *or* in the mixed state of knowledge represented by (11.3). But we do claim that if we should fail to observe particles in classical motion in the regions where they might be expected, then this 'null measurement' should lead us to adopt the array (11.3) to represent our revised mixed state of knowledge.

The theory of part-quasi-classical mixed states of knowledge will be of importance in connection with the realisation of pure states (in the next section).

12. The acquisition of pure states of knowledge

In our interpretation of quantum mechanics we have claimed that it is always possible, in principle, for us to be in a pure state of knowledge (regarding the dynamical properties of a quantum mechanical system) represented by any one wave function specified to within an arbitrary constant phase factor. For completeness, we need to show *how* this is possible. We can do this by modelling preparation processes that assume only easily acquired (non-pure) prior knowledge of a system's dynamics but demonstratively result in (posterior) pure knowledge of the system's dynamics. We give examples below. Of course, in these examples, and generally, pure states are *ideal* states of knowledge that can never be exactly realised, but only realised to 'quantum mechanical accuracy'.

Since a wave function changes (according to the Schrödinger equation) whenever the system in question moves under the action of a known inter-particle potential and known external fields, there are (over time) very many wave functions associated with the same pure state of knowledge. Therefore, having realised a particular wave function (for example the wave function representing knowledge of a particle's momentum at one time) we have, in time, realised every wave function into which the original wave function evolves in given external fields. Indeed, having realised any one wave function referring to one time, we may assume that any other wave function for the same system may be eventually realised if only the external fields to which the system is subjected are suitably chosen. So it is sufficient to show how to realise any *one* ('primary') wave function of a system (referring to a basic set of properties at one time) in order to show that *any* wave function for that system could be realised.

We give below only methods for realising 'primary' wave functions for a *single* particle. But of course, using the methods to be described, primary wave functions for several particles might be realised simultaneously and independently (in different regions of space) to give multi-particle wave functions *separable* into single particle wave functions. And then, by letting the particles move in external fields and interact with each other under supposed known time-dependent inter-particle potentials, we might (in principle) realise any *inseparable* multi-particle wave function.

12.1 Preparation of a pure state of knowledge of a particle's position

Suppose we know only that the particle is enclosed (on its own) in a 'box' as defined in section 3.1.1 of Chapter XI. This is arguably a *feasible* initial state of knowledge to be in from a practical point of view, and for convenience we take the sides of the box to be of equal length.

By the third law of array assignment (section 6) our mixed state of knowledge is represented by an array containing any complete set of (allowed) orthogonal wave functions and equal weights. Taking the wave functions to be those in (3.1.1.1) of

Chapter XI labelled by the ordered integers (n_1, n_2, n_3) each going from 1 to N (and letting $N \rightarrow \infty$ eventually) the array representing our initial knowledge can be written

$$\left\{ \dots, \phi_{n_1 n_2 n_3}(x, y, z), \dots ; \dots, w_{n_1 n_2 n_3}, \dots \right\} \quad (12.1.1)$$

where the weights $w_{n_1 n_2 n_3}$ are all equal.

To avoid having to take the limit as $N \rightarrow \infty$ we might instead assume we know that (i) the particle is in the box *and* (ii) its kinetic energy is (for all time) less than a certain value E_0 . This is arguably also a feasible initial state of knowledge. Then, claiming this state of knowledge qualifies as a ‘mixed state’ and noting that this state of knowledge is time independent, we can argue (in the way we did in section 8.1) that the stationary state wave functions $\phi_{n_1 n_2 n_3}(x, y, z)$ may be employed in the array representing our mixed state of knowledge. The weights in our array can then be found by applying the *second* law of array assignment, our constraints on the weights being

$$w_{n_1 n_2 n_3} = 0, \text{ for } E_{n_1 n_2 n_3} \geq E_0 : \text{ and } \sum_{n_1 n_2 n_3} w_{n_1 n_2 n_3} = 1. \quad (12.1.2)$$

The second of these is straightforward normalisation. The first is a consequence of the general law of probability of a parametric property (see (2.1.2)) and the fact that the kinetic energy is known to be greater than or equal to E_0 . Since the energy $E_{n_1 n_2 n_3}$ associated with $\phi_{n_1 n_2 n_3}(x, y, z)$ is (by (3.1.1.3) of Chapter XI) proportional to the sum of the squares of n_1, n_2 and n_3 (the sides of the box being equal), the first constraint amounts to the requirement that the weights $w_{n_1 n_2 n_3}$ are zero for points (n_1, n_2, n_3) (in a representative 3-D space) lying outside a certain sphere whose centre is at the origin. Let the number of such points lying *within* the sphere be N_0 . Then the information entropy in the second law of array assignment is maximised when the N_0 weights (one for each representative point within the sphere) are all equal. So our array has the same form as in (12.1.1) except that the number N_0 of wave functions $\phi_{n_1 n_2 n_3}(x, y, z)$, and of weights $w_{n_1 n_2 n_3}$, is finite, each weight being equal to $\frac{1}{N_0}$, and the wave functions (and weights) are of course limited to those for which the points (n_1, n_2, n_3) in 3-D representative space lie inside the sphere.

To prepare the particle so that we have a pure state of knowledge of its position we can proceed as follows.

At time t let the external potential providing the ‘walls’ of the box be ‘switched off’ and let us, at the same time, attempt, by the method of section 2.2 of Chapter XIII, to locate the particle position at a point (x_0, y_0, z_0) at which none of the $\phi_{n_1 n_2 n_3}$ in (12.1.1) vanish. Accordingly, we apply, within the box (from time t to time $t + \delta$) and in all but a vanishingly small region around (x_0, y_0, z_0) , a scalar potential with a large gradient k in

the x direction, taking the limit as $k \rightarrow \infty$ and $\delta \rightarrow 0$ while $k\delta$ remains finite and large and then the limit $k\delta \rightarrow \infty$ as the small region around (x_0, y_0, z_0) becomes a (quantum mechanical) infinitesimal. Then, if no particle in classical motion is observed far away shortly after time t we establish, harmlessly with regard to particle position, that the particle is at (x_0, y_0, z_0) at time t . That is, we establish a wave function

$$\psi(x, y, z) = \delta(x - x_0)\delta(y - y_0)\delta(z - z_0) \quad (12.1.3)$$

expressing our (now pure) state of knowledge that the particle is at (x_0, y_0, z_0) .

That this method will work, i.e. will result in a pure state of knowledge represented by (12.1.3), follows from the law of natural evolution of an array representing a mixed state of knowledge (section 1) and from the law of part-quasi-classical mixed states (section 11). By the first law, each wave function in our array evolves according to the Schrödinger equation while the weights remain constant. In the short time from t to time $t + \delta$, therefore, each wave function $\phi_{n_1 n_2 n_3}(x, y, z)$ in our initial array (12.1.1) evolves into a part-quasi-classical form:

$$\Psi_{n_1 n_2 n_3}(x, y, z) = k_{n_1 n_2 n_3}^{(0)} \delta(x - x_0)\delta(y - y_0)\delta(z - z_0) + k_{n_1 n_2 n_3}^{(qc)} \phi'_{n_1 n_2 n_3}(x, y, z) \quad (12.1.4)$$

where $\phi'_{n_1 n_2 n_3}(x, y, z)$ is a normalised quasi-classical wave function of the form of a fast travelling wave packet soon enough far away (far away from the region of space initially occupied by the box), and the k s are non-zero complex constants. If we observe no classical particle far away (in the region of space where the $\phi'_{n_1 n_2 n_3}(x, y, z)$ have significant value, then, by the law of part-quasi-classical mixed states of knowledge, the array representing our knowledge collapses to

$$\left\{ \dots, \delta(x - x_0)\delta(y - y_0)\delta(z - z_0), \dots; \dots, P_{n_1 n_2 n_3} W_{n_1 n_2 n_3}, \dots \right\} \quad (12.1.5)$$

where the wave functions are all the same. Regardless of the values of the weights in (12.1.5), this array represents a pure state of knowledge of particle dynamics with wave function given by (12.1.3) to within a constant phase factor (see section 2.3). So we have, in principle, achieved what we set out to do.

12.2 Preparation of a pure state of knowledge of a particle's spin component

Let the particle have spin s so that its z component of spin (in a fixed coordinate system O) takes one of the $2s + 1$ values $\sigma = -s, -s + 1, \dots, s$.

Suppose we know initially, as in section 12.1, that (i) the particle is in a box *and* (ii) its kinetic energy is (for all time) less than a certain value E_0 . And suppose we know (iii) that there is no external magnetic field, and we know nothing about the z component of the particle's spin. We again claim we are in a mixed state of knowledge (in relation to

closed sample space $S_{r\sigma}$ which is the combination of closed sample spaces S_r and S_σ , and since this is knowledge that remains the same in time, the array representing our knowledge may employ a complete set of orthogonal stationary wave functions of the system. We thus take the wave functions to be $\phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma n_4}$ where the $\phi_{n_1 n_2 n_3}(x, y, z)$ are as in section 12.1 and n_4 is a new parameter taking values $-s, -s+1, \dots, s$. Applying the second law of array assignment we have (in a way very similar to that in section 12.1) that the array representing our knowledge has the form

$$\left\{ \dots, \phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma n_4}, \dots; \dots, \frac{1}{N_0(2s+1)}, \dots \right\} \quad (12.2.1)$$

where the weights are all equal and are now $N_0(2s+1)$ in number.

We note that the array (12.2.1) factors (in the sense of section 3) and therefore represents a state of knowledge the same as having a mixed state of knowledge in S_r with array

$$\left\{ \dots, \phi_{n_1 n_2 n_3}(x, y, z), \dots; \dots, \frac{1}{N_0}, \dots \right\} \quad (12.2.2)$$

and a mixed state of knowledge in S_σ with array

$$\left\{ \dots, \delta_{\sigma n_4}, \dots; \dots, \frac{1}{(2s+1)}, \dots \right\} \quad (12.2.3)$$

the weights in each array being equal among themselves.

To prepare the particle so that we have a pure state of knowledge in S_σ regarding its spin component, we can proceed as follows.

At time t let the external potential providing the ‘walls’ of the box be ‘switched off’ and let us attempt to instantly establish that the particle’s z component of spin in O has some particular value σ_0 by employing the method of section 3.1 of Chapter XIII.

That method requires us to apply (from time t to time $t+\delta$) a magnetic field in the z direction with a gradient k in the x direction. We take the limit as $k \rightarrow \infty$ and $\delta \rightarrow 0$ while $k\delta$ remains finite and large. This will cause wave functions $\phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma n_4}$ for which $n_4 \neq 0$ to move (as wave packets $\phi'_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma n_4}$) rapidly in the x direction into regions far off (wave functions $\phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma n_4}$ with the same value of n_4 sharing the same region). If we are seeking to establish that $\sigma=0$ (i.e. if $\sigma_0=0$) we apply no more impulsive fields. But if we are seeking to establish that $\sigma=\sigma_0$ where $\sigma_0 \neq 0$, we apply, immediately after the magnetic impulse, an ordinary potential gradient impulse to the wave functions $\phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_0}$ (which have not been moved by our magnetic impulse), to send *them* off to infinity in a different direction. Now, when $\sigma_0 \neq 0$, we apply to the region occupied by the wave functions $\phi'_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_0}$ and to no other region, a magnetic field gradient impulse of opposite sign and twice as great as

that initially applied. This will send those wave functions back to the region where the box was situated and as they arrive back we bring them to rest by applying a final magnetic field gradient impulse equal to that first applied. The result (whether or not $\sigma_0 = 0$) is that the wave functions $\phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_0}$ are returned to their original forms while the others (those for which $n_4 \neq \sigma_0$) are sent flying.

The array (12.2.1) representing our initial state of knowledge accordingly changes to one with the same weights (all equal) but with the following wave functions. We have N_0 ordinary wave functions $\phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_0}$ which are the same as they were in (12.2.1) and $N_0 \cdot 2s$ wave functions $\phi'_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_{n_4}}$ (where $n_4 \neq \sigma_0$) which are now flying wave packets far away (see section 3.1 of Chapter XIII). We write this array as

$$\left\{ \dots, \phi'_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_{n_4}}, \dots, \phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_0}, \dots; \dots, \frac{1}{N_0(2s+1)}, \dots \right\} \quad (12.2.4)$$

where, for convenience, all the wave packet wave functions come first and all the ordinary (returned) wave functions come after.

Array (12.2.4) represents a part-quasi-classical mixed state of knowledge (section 11) in which some of the wave functions are ordinary wave functions and some are quasi-classical wave functions carrying the definite spin component value σ_0 . We accordingly know the particle is moving (to classical accuracy) in one or other of the classical paths associated with the quasi-classical wave functions $\phi'_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_{n_4}}$ (where $n_4 \neq \sigma_0$), as under the mixed state of knowledge represented by the array

$$\left\{ \dots, \phi'_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_{n_4}}, \dots; \dots, \frac{1}{N_0 \cdot 2s}, \dots \right\} \quad (n_4 \neq \sigma_0) \quad (12.2.5)$$

or the particle is somewhere in the region where it was initially under the mixed state of knowledge represented by the array

$$\left\{ \dots, \phi_{n_1 n_2 n_3}(x, y, z)\delta_{\sigma_0}, \dots; \dots, \frac{1}{N_0}, \dots \right\}. \quad (12.2.6)$$

Our degrees of belief for these alternatives are (by (11.5)) the relative number of wave packet wave functions in (12.2.4) and the relative number of non-wave-packet wave functions in (12.2.4). These are respectively the same as the relative numbers of associated spin components, i.e. $\frac{2s}{2s+1}$ and $\frac{1}{2s+1}$.

If we fail to observe, just after time t , a particle in classical motion far away, the array representing our mixed state of knowledge collapses from (12.2.4) to (12.2.6), (see the end of section 11). Further, our collapsed array (12.2.6) factors into mixed state array

$$\left\{ \delta_{\sigma_0}; 1 \right\} \quad (12.2.7)$$

in S_{σ_0} , and mixed state array

$$\left\{ \dots, \phi_{n_1 n_2 n_3}(x, y, z), \dots; \dots, \frac{1}{N_0}, \dots \right\} \quad (12.2.8)$$

in S_r . The first represents a pure state of knowledge now held in S_σ , namely knowledge that the z component of spin of the particle is σ_0 . So we have achieved what we set out to do. The second array represents a mixed state of knowledge now held in S_r which is just the mixed state that would apply had we disregarded our knowledge that the particle has spin. Clearly we may now switch back on the potentials providing the walls of the box and hold (after time t) the pure state of knowledge represented by the array (12.2.7) in S_σ and the mixed state of knowledge represented by the array (12.2.8) in S_r .

12.3 Preparation of a pure state of knowledge of a particle's momentum

We now model a method for preparing a particle (mass m) so that when the particle moves freely after time $t=0$ we hold (pure) knowledge (in the sample space S_r) of its constant momentum \mathbf{p} relative to a fixed coordinate system O . The following method is related to the heuristic procedure used by Feynman and Hibbs (p. 97 of [16]) for deriving the wave function in the momentum representation from the wave function in the position representation.

Let \mathbf{r}_0 denote a position in our fixed coordinate system O related to the required momentum \mathbf{p} by $\mathbf{p} = -m\mathbf{r}_0/r_0$. So the vector \mathbf{r}_0 points (from the origin) in a direction opposite to that of \mathbf{p} . At time $t_0 = -mr_0/p$ let us suppose we have located the particle at \mathbf{r}_0 so that at time t_0 we are in a pure state of knowledge of its position represented by the wave function

$$\delta(\mathbf{r} - \mathbf{r}_0). \quad (12.3.1)$$

We can do this using the method given in section 12.1.

Allowing the particle to move freely after time t_0 our wave function at time t (with $t > t_0$) is, by (1.20) of Chapter IV

$$\phi_{r_0 t_0}(\mathbf{r}, t) = \left(\frac{2\pi i \hbar (t - t_0)}{m} \right)^{-3/2} \exp i \left(\frac{m(\mathbf{r} - \mathbf{r}_0)^2}{2\hbar(t - t_0)} \right) \quad (12.3.2)$$

where α has been put equal to its known value of $\frac{1}{2}$. More correctly, our wave function $\psi(\mathbf{r}, t)$ is, by the first of (1.2) of Chapter IV,

$$\psi(\mathbf{r}, t) = \phi_{r_0 t_0}(\mathbf{r}, t) \sqrt{\Delta V} \quad (12.3.3)$$

where ΔV is the volume element at \mathbf{r}_0 in which we initially located the particle. (Ideally $\Delta V \rightarrow 0$ or rather ΔV is an infinitesimal.)

Now at time $t=0$ let us suppose we establish, by harmless conditioning (as in section 2.1 of Chapter XIII) that the particle is inside a volume V of space containing the origin of our coordinates. We will suppose point \mathbf{r}_0 is so far away from V that V subtends a small solid angle from \mathbf{r}_0 . But, be this as it may, our wave function (12.3.2) collapses to

$$\psi(\mathbf{r},0) = \begin{cases} \frac{\phi_{\mathbf{r}_0 t_0}(\mathbf{r}0)\sqrt{\Delta V}}{\sqrt{\int_V |\phi_{\mathbf{r}_0 t_0}(\mathbf{r}0)|^2 \Delta V d^3\mathbf{r}}} e^{-ik} & \mathbf{r} \text{ in } V \\ 0 & \mathbf{r} \text{ outside } V \end{cases} \quad (12.3.4)$$

(cf. (4.2) of Chapter II) where k is the phase characteristic of our knowledge that the particle is at \mathbf{r}_0 at time t_0 and β is our phase of belief that under the same knowledge the particle is in V at time $t=0$. Of course k , β and $-k-\beta$ are indeterminate.

By (12.3.2)

$$\int_V |\phi_{\mathbf{r}_0 t_0}(\mathbf{r}0)|^2 d^3\mathbf{r} = \left(\frac{2\pi\hbar m r_0/p}{m}\right)^{-3} V.$$

And (12.3.4) becomes

$$\psi(\mathbf{r},0) = \begin{cases} V^{-1/2} i^{-3/2} \exp i\left(\frac{m(\mathbf{r}-\mathbf{r}_0)^2}{2\hbar m r_0/p} - k - \beta\right) & \mathbf{r} \text{ in } V \\ 0 & \mathbf{r} \text{ outside } V \end{cases} \quad (12.3.5)$$

Now in (12.3.5)

$$\frac{m(\mathbf{r}-\mathbf{r}_0)^2}{2m r_0/p} = p \frac{(\mathbf{r}-\mathbf{r}_0)^2}{2r_0} = \frac{1}{2} p \frac{r^2 - 2\mathbf{r}\cdot\mathbf{r}_0 + r_0^2}{r_0},$$

and since $\mathbf{p} = -p\mathbf{r}_0/r_0$, we have, in (12.3.5) that

$$\frac{m(\mathbf{r}-\mathbf{r}_0)^2}{2\hbar m r_0/p} = \frac{1}{\hbar} \mathbf{p}\cdot\mathbf{r} + \frac{1}{2\hbar} p \frac{r^2 + r_0^2}{r_0}. \quad (12.3.6)$$

The second term on the RHS of (12.3.6) represents (in (12.3.5)) an unimportant constant phase factor $\frac{1}{2} p r_0/\hbar$ plus a phase factor $\frac{1}{2} p r^2/r_0\hbar$ which is $\ll 1$ for all \mathbf{r} in V provided

r_0 is chosen large enough, and accordingly t_0 made large enough so that $p (= -mr_0/t_0)$ remains the same. If D is the dimension of V (so that $V \approx D^3$) we make

$$D \gg \frac{\hbar}{p} \quad \text{and} \quad \frac{1}{2\hbar} p \frac{D^2}{r_0} \ll 1.$$

The first is to ensure there are very many de Broglie wavelengths within V and the second is to ensure $\frac{1}{2} p r^2 / r_0 \hbar$ is $\ll 1$. The two requirements are together equivalent to

$$D \gg \frac{\hbar}{p} \gg \frac{1}{2} \frac{D^2}{r_0} \tag{12.3.7}$$

which can be met (for any aimed-at-value of p) by first making D large enough compared to \hbar/p and then making r_0 large enough in comparison to D (with t_0 chosen so that $mr_0/t_0 = p$).

Then, in V , we have from (12.3.5) and (12.3.6) that

$$\psi(\mathbf{r},0) = V^{-1/2} \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar - i\gamma) \tag{12.3.8}$$

where γ is an indeterminate constant phase. Allowing V to tend to infinity (as we have seen we may) (12.3.8) has the same form as the derived ideal wave function representing knowledge that the momentum \mathbf{p} lies in an infinitesimal element $d^3\mathbf{p}$ of momentum space, i.e. the same form as the wave function

$$\psi(\mathbf{r},0) = (2\pi\hbar)^{-3/2} \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar) \sqrt{d^3\mathbf{p}} .$$

See the first of (3.10) of Chapter VI where the indeterminate constant phase factor was conventionally taken as 1. So we have achieved a pure state of knowledge of the particle's momentum.

THE RESOLUTION OF PARADOXES

The interpretation of quantum mechanics we offer in the present work is not a hidden-variables theory in the sense that we provide laws that certain hidden variables must follow and deduce the formalism of quantum mechanics from these laws using classical probability theory. It is however a hidden-variables theory in the sense that we take all properties (as represented, in the usual formalism, by complete sets of commuting observables in component Hilbert spaces) to have definite (usually hidden) values. (So, for example, the position of a particle is considered to exist objectively and its momentum too is considered to exist objectively, and so on. The position vector \mathbf{r} and momentum vector \mathbf{p} of each particle in a particle system are thus assumed to have definite values at any time regardless of any knowledge we may or may not have of the system dynamics.) We do not claim to know the detailed laws of evolution of properties but instead claim to know only certain general laws governing their evolution (such as the possibility of time-reversal). And on the basis of this limited knowledge we deduce the equations of the usual quantum mechanical formalism using a new (rational-Bayesian) probability theory.

Now various arguments have been put forward to show that hidden-variables theories (of any kind) are untenable; that they are not consistent with the usual formalism of quantum mechanics. In this Chapter we consider some of these arguments in order to show that they are not providing reasons why the *present interpretation* must be inconsistent.

1. The Kochen-Specker paradox

Accounts of the Kochen-Specker paradox are given by Belinfante [26] and Redhead [4]. In its general form (section 3.5 of [26]), and in our notation, the Kochen-Specker paradox relates to sets of orthogonal wave functions $\Phi(x_i|P_j)$ of the kind discussed in section 3.12 of Chapter I in connection with the law of general dynamical properties and associated probabilities. We claimed there that to any complete set of orthogonal wave functions $\Phi(x_i|P_j)$ ($j=1,\dots,N$) of unspecified absolute phase there corresponds a dynamical property P of our system S quantified by j ($j=1,\dots,N$), and each state of knowledge P_j (associated with the wave function $\Phi(x_i|P_j)$) is represented by proposition P_j claiming that P is quantified by j . And in the expansion of any wave function $\Phi(x_i|Y)$ in the $\Phi(x_i|P_j)$, i.e. in

$$\Phi(x_i|Y) = \sum_j a_j \Phi(x_i|P_j) \quad (1.1)$$

the squared moduli of the coefficients give the degrees of belief we should hold for P being quantified by j under knowledge Y , so that

$$|\Phi(P_j|Y)|^2 = |a_j|^2. \quad (1.2)$$

Now to derive the Kochen-Specker paradox we need to suppose that:

If P_j ($j=1,\dots,N$) and P'_k ($k=1,\dots,N$) are properties of S corresponding to two complete sets of orthogonal wave functions $\Phi(x_i|P_j)$ and $\Phi(x_i|P'_k)$ (of indeterminate absolute phase) which share a common member, so that for a particular value of j and a particular value of k

$$\Phi(x_i|P_j) = \Phi(x_i|P'_k) e^{i\beta} \text{ for all } i \quad (1.3)$$

(β being some constant phase) then (for that particular value of j and that particular value of k)

$$P_j \Leftrightarrow P'_k. \quad (1.4)$$

That is, under relation (1.3), and under our general knowledge G , proposition P_j (claiming P is quantified by j) implies proposition P'_k (claiming P' is quantified by k) and vice versa, independently of any knowledge we may or may not hold with regard to the dynamical properties of the system S .*

Under this supposition a contradiction arises. For we may picture the wave functions $\Phi(x_i|P_j)$ and the wave functions $\Phi(x_i|P'_k)$ as orthogonal sets of unit vectors from the origin of a function space of dimension N , and under any state of knowledge Y in S (pure or not) can imagine each vector of the set $\Phi(x_i|P_j)$ to be labelled 1 or 0 according as P is (under knowledge Y) in fact quantified by j or not. And we can

* We would naturally take this to be true if we were to regard wave functions as representing states of the system under given physical conditions rather than probability distributions going with states of our knowledge. Then (1.3) would imply the same state of the system accompanied properties P_j and P'_k . So when property P_j is present state $\Phi(x_i|P_j)$ is present and therefore property P'_k is present also. (For if P'_l (with $l \neq k$) was present instead the system would be in state $\Phi(x_i|P'_l)$ different from the state $\Phi(x_i|P_j)$.)

imagine similar labelling applied to the set of vectors $\Phi(x_i|P'_k)$ or $\Phi(x_i|P''_k)$...etc. formed by rotating the set $\Phi(x_i|P_j)$ (as a whole) in function space in any manner we please*. Then, of course, whenever the set $\Phi(x_i|P'_k)$ shares a common member with another set $\Phi(x_i|P''_k)$ there would be need, on account of result (1.4), to assign the *same* value (1 or 0) to the shared vector. But such labelling of vectors in a function space is precisely what Kochen and Specker have shown to be impossible for $N \geq 3$.

However, in the present interpretation of quantum mechanics, (1.4) does not follow from (1.3). We *can* show (as done in section 6.3 of Chapter II), that for the particular value of j and the particular value of k for which (1.3) applies

$$\Phi(P_j|P'_k) = e^{-i\alpha} \quad \text{and} \quad \Phi(P'_k|P_j) = e^{-i\gamma}$$

where α and γ are *indeterminate* phases. But by the first law of extreme values of probability, it follows from this (as explained in section 6.3 of Chapter II) only that the *acquisition of knowledge* of the truth of P'_k (or of P_j) by measurement or system preparation brings about or ensures the truth of P_j (or of P'_k respectively). Ordinarily, the properties P_j and P'_k do not necessarily occur together. So the Kochen-Specker paradox does not arise because, in the proposed labelling, the common vectors from sets $\Phi(x_i|P_j)$ ($j = 1, \dots, N$) and $\Phi(x_i|P'_k)$ ($k = 1, \dots, N$) need not be assigned the same value (1 or 0).

In the present interpretation of quantum mechanics we are thus free to claim that all properties have definite values without giving rise to the Kochen-Specker paradox.

2. Nonlocality and Bell's theorem

Bell's theorem (or Bell's inequality) has been much discussed in the literature on the interpretation of quantum mechanics and formulated in different ways (see for example Chapter 4 of [4]). It relates to measurements made by two observers widely separated from each other in space each measuring spin components of one of the two spin one-half particles emerging from a source (midway between the observers) in a 'singlet spin state'. And it shows why certain general kinds of local-action statistical hidden-variables theories cannot account for the measurements made by the observers in repeated experiments. Certain statistical correlations between their measurements (predicted by the quantum theory and confirmed in practice) are shown to be necessarily different from the statistical correlations that any hidden-variables theory of the kind considered could come up with.

This has led some to the conclusion that a measurement of a spin component of one particle must instantly change a spin component of the other even though the particles may be as far away from each other as we please. Only in that way, they reason,

* This assumes any such rotation results in orthogonal functions that qualify as wave functions as is very often the case.

could the observed correlations be realistically explained. To these people (instant) ‘action at a distance’* or ‘nonlocality’ is sometimes present in quantum mechanical processes.

In the present interpretation of quantum mechanics Bell type inequalities are not derivable because they employ classical probability which according to us does not apply at the quantum mechanical level. The classical laws of probability are not expected to apply to the probability distributions over quantum mechanical variables (like spin components) or to hidden-variables that might be associated with processes occurring at a deeper level. Accordingly we are not led to the belief in (instant) ‘action at a distance’ or ‘nonlocality’.

It is of interest however to consider what the present interpretation of quantum mechanics has to say about some of the mathematical relations that arise in connection with measurements performed on a system of the kind envisaged by Bell.

2.1 The system considered with measurements viewed as harmless conditioning

We suppose, with Bell, that somehow a system composed of two non-identical spin one-half particles 1 and 2 is prepared (set moving in free space) in a way that leads to our state of knowledge of its dynamical properties being represented, at any time (from time t_0 onward), by a wave function in sample space $S_{r_1 r_2} S_{\sigma_1 \sigma_2}$ of the form

$$\frac{1}{\sqrt{2}} \phi_A(\mathbf{r}_1, t) \phi_B(\mathbf{r}_2, t) (\delta_{\sigma_1 \frac{1}{2}} \delta_{\sigma_2 -\frac{1}{2}} - \delta_{\sigma_1 -\frac{1}{2}} \delta_{\sigma_2 \frac{1}{2}}) \quad (2.1.1)$$

$\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2$ being the positions and z components of spin of the particles in a fixed Cartesian coordinate system O , and ϕ_A, ϕ_B normalised functions describable as separate wave packets moving away from the origin of O in opposite directions along the x axis of the coordinates. Since this wave function is a product of a function of $\mathbf{r}_1, \mathbf{r}_2$ and a function of σ_1, σ_2 , and since $S_{r_1 r_2}$ and $S_{\sigma_1 \sigma_2}$ are each closed sample spaces, our knowledge separates into pure knowledge in relation to the orbital motion of the particles and pure knowledge Y relating to the spinning motion of the particles. And henceforth we speak theoretically only about our knowledge of the spinning motions, and we refer only to propositions in the sample space $S_{\sigma_1 \sigma_2}$.

Our wave function in $S_{\sigma_1 \sigma_2}$ is

$$\Phi(\sigma_1 \sigma_2 t | Y) = \frac{1}{\sqrt{2}} (\delta_{\sigma_1 \frac{1}{2}} \delta_{\sigma_2 -\frac{1}{2}} - \delta_{\sigma_1 -\frac{1}{2}} \delta_{\sigma_2 \frac{1}{2}}) e^{i\alpha} \quad (2.1.2)$$

where α is an indeterminate constant phase. Since there is no magnetic field, the Hamiltonian in (4.3) of Chapter VIII is zero so wave function (2.1.2) is independent of

* an action that, notably, cannot be used to communicate messages

time. And the component pair $\sigma_1\sigma_2$ (i.e. the values of σ_1 and σ_2) are *naturally constant in time* because the Schrödinger equation gives the result that the proposition ‘ $\sigma_1\sigma_2 = \frac{1}{2} - \frac{1}{2}$ at time t_0 ’ for example (which can be used to express a pure state of knowledge with wave function $\Phi(\sigma_1\sigma_2|t|_{\frac{1}{2}-\frac{1}{2}t_0}) = \delta_{\sigma_1\frac{1}{2}}\delta_{\sigma_2-\frac{1}{2}}$) implies ‘ $\sigma_1\sigma_2 = \frac{1}{2} - \frac{1}{2}$ at time t ’ (for any t greater than t_0) with a determinate phase of implication (namely zero) and therefore regardless of any knowledge we may or may not hold about the spinning motions; and similar remarks apply with regard to all other values of $\sigma_1\sigma_2$.

Theoretically, the basis $\sigma_1\sigma_2$ is a primary basis so it is possible to perform harmless conditioning in $S_{\sigma_1\sigma_2}$. We suppose therefore that at some time $t' > t_0$ (when the particles are far apart) we harmlessly get to know the spin component σ_1 , finding that it is in fact $\frac{1}{2}$. A question of interest is what does this tell us about σ_2 in the sample space $S'_{\sigma_1\sigma_2}$ following our harmless conditioning? To answer this question, we start by working out the probabilities for the possible values of σ_2 after we got to know that σ_1 was $\frac{1}{2}$.

From the general result (4.2) of Chapter II, our wave function in $S'_{\sigma_1\sigma_2}$ just after the harmless conditioning at time t' is

$$\Phi(\sigma_1\sigma_2|\sigma_1 = \frac{1}{2} Y) = \begin{cases} \frac{\Phi(\sigma_1\sigma_2|Y)}{\Phi(\sigma_1 = \frac{1}{2}|Y)} e^{-ik} & \sigma_1 = \frac{1}{2} \\ 0 & \sigma_1 \neq \frac{1}{2} \end{cases} \quad (2.1.3)$$

where k is the phase characteristic of our (initial) knowledge Y and, by the sum rule

$$\Phi(\sigma_1 = \frac{1}{2}|Y) = e^{i(\chi-k)} \sqrt{|\Phi(\frac{1}{2}\frac{1}{2}|Y)|^2 + |\Phi(\frac{1}{2}-\frac{1}{2}|Y)|^2} = \frac{1}{\sqrt{2}} e^{i(\chi-k)} \quad (2.1.4)$$

where χ is the phase characteristic of proposition $\sigma_1 = \frac{1}{2}$ under knowledge Y .

Substituting (2.1.4) and (2.1.2) into (2.1.3) we find

$$\Phi(\sigma_1\sigma_2|\sigma_1 = \frac{1}{2} Y) = \delta_{\sigma_1\frac{1}{2}} \delta_{\sigma_2-\frac{1}{2}} e^{-i(\chi-\alpha)} \quad (2.1.5)$$

and, because this is a product of a function of σ_1 and a function of σ_2 and the sample spaces S'_{σ_1} and S'_{σ_2} are closed, our knowledge splits into pure knowledge in S'_{σ_1} referring to particle 1 and pure knowledge in S'_{σ_2} referring to particle 2.

Applying (as we clearly may) the general result (1.4.4) of Chapter II to (2.1.5) with $\sigma_1 = \frac{1}{2}$ we should put for our wave function in S'_{σ_2} with our pure knowledge expressed as $\sigma_1 = \frac{1}{2} Y$:

$$\Phi(\sigma_2 | \sigma_1 = \frac{1}{2} Y) = \delta_{\sigma_2 - \frac{1}{2}} e^{-i(\chi - \alpha + \varepsilon)} \quad (2.1.6)$$

where ε is the phase characteristic of knowledge $\sigma_1 = \frac{1}{2}$. Here χ, α and ε are indeterminate and unrelated constant phases, and the total phase $\chi - \alpha + \varepsilon$ in (2.1.6) is also indeterminate. Also, on account of the general rule (2.2.1.21) of Chapter I, we should put for our wave function in S'_{σ_1} with our knowledge expressed in the same way:*

$$\Phi(\sigma_1 | \sigma_1 = \frac{1}{2} Y) = \delta_{\sigma_1 - \frac{1}{2}} e^{-ik} \quad (2.1.7)$$

Since there is no magnetic field, wave functions (2.1.6) and (2.1.7) hold for all times greater than t' and by the natural conservation of spin components in the absence of a magnetic field, $\sigma_1 = \frac{1}{2}$ and $\sigma_2 = -\frac{1}{2}$ are necessarily true for all times greater than t' .

Now on account of the indeterminate phase factor in (2.1.6) the first and second laws of extreme values of probability suggest that the acquisition of knowledge Y and then of knowledge $\sigma_1 = \frac{1}{2}$ at time t' physically brings about or ensures the property $\sigma_2 = -\frac{1}{2}$ thereafter. (And by a similar argument the acquisition of knowledge Y and then of knowledge $\sigma_1 = -\frac{1}{2}$ at time t' would physically bring about or ensure the property $\sigma_2 = \frac{1}{2}$ thereafter). Now we know, as we have said, that (on account of $\sigma_1 \sigma_2$ being a primary basis) we can (as in (2.1.6)) get to know the value of σ_1 without affecting the value of σ_2 or of σ_1 itself. So it would have to be that the acquisition of knowledge Y alone was sufficient to ensure opposite spin components. That this is in fact the case (i.e. that opposite spins are ensured after acquiring knowledge Y alone) may be directly confirmed as follows.

We calculate the wave function (under knowledge Y) using the basis $s\sigma$ of total spin s and its z component σ . This is done by transforming $\Phi(\sigma_1 \sigma_2 t | Y)$ to $\Phi(s\sigma t | Y)$ using the transformation function in (3.5) of Chapter VIII. This gives, in the matrix notation

* Note that by the product rule for wave functions, the product of (2.1.6) and (2.1.7) should be the wave function $\Phi(\sigma_1 \sigma_2 | (\sigma_1 = \frac{1}{2} Y)(\sigma_1 = \frac{1}{2} Y))$ in $S'_{\sigma_1 \sigma_2}$. Since, by (1.3) of Chapter II,

$(\sigma_1 = \frac{1}{2} Y)(\sigma_1 = \frac{1}{2} Y) \stackrel{\gamma}{\Leftrightarrow} (\sigma_1 = \frac{1}{2} Y)$ with $\gamma = \varepsilon + k$, this is in agreement with (2.1.5).

$$\Phi(s\sigma t|Y) = \sum_{\sigma_1\sigma_2} \Phi(s\sigma|\sigma_1\sigma_2)\Phi(\sigma_1\sigma_2 t|Y) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} 0 \\ e^{i\alpha/\sqrt{2}} \\ -e^{i\alpha/\sqrt{2}} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ e^{i\alpha} \end{pmatrix}$$

Therefore, conversely, under supposed pure knowledge $Z = 's=0$ and $\sigma=0$ at time t_0 ', we find

$$\Phi(\sigma_1\sigma_2 t|Z) = \sum_{s\sigma} \Phi(\sigma_1\sigma_2|s\sigma)\Phi(s\sigma t|Z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{pmatrix}$$

which apart from a constant phase factor is the same wave function as (2.1.2). And because of the 1-1 correspondence (to within a constant phase factor) between wave functions (in basis $\sigma_1\sigma_2$) and pure states of knowledge of system dynamics, pure knowledge Z is the same as pure knowledge Y . That is, we can be certain that $\sigma_1 = -\sigma_2$ under knowledge Y , and we can indeed claim that acquisition of knowledge Y brings about or ensures the truth of the equality $\sigma_1 = -\sigma_2$ from time t_0 onwards.

2.2 The Bell-Wigner inequality and its implications

We now consider an inequality that goes with Bell's theorem but is more direct than the original Bell inequality in that it involves *probabilities* of spin component measurement results rather than *correlations* between such measurements. This 'new' inequality is due to Wigner and is described for example in section 6.7 of [30].

In connection with the process of section 2.1, we now work in an alternative basis $\sigma'_1\sigma''_2$ where σ'_1 and σ''_2 are the z components of spin of particles 1 and 2 in stationary coordinates O' and O'' respectively which share their x axes with the x axis of the original coordinates O but have their z axes rotated about the x axis through angles α' and α'' respectively.

To obtain the wave function $\Phi(\sigma'_1\sigma''_2|Y)$ which corresponds to wave function (2.1.2) in the original basis we need the transformation function $\Phi(\sigma'_1\sigma''_2|\sigma_1\sigma_2)$ which will be the product of the transformation functions $\Phi(\sigma'_1|\sigma_1)$ and $\Phi(\sigma''_2|\sigma_2)$ given, in the matrix notation, by

$$\Phi(\sigma'_1|\sigma_1) = \begin{pmatrix} \cos \frac{\alpha'}{2} & i \sin \frac{\alpha'}{2} \\ i \sin \frac{\alpha'}{2} & \cos \frac{\alpha'}{2} \end{pmatrix}, \quad \Phi(\sigma''_2|\sigma_2) = \begin{pmatrix} \cos \frac{\alpha''}{2} & i \sin \frac{\alpha''}{2} \\ i \sin \frac{\alpha''}{2} & \cos \frac{\alpha''}{2} \end{pmatrix} \quad (2.2.1)$$

as follows from the general transformation function in (3.5) and (5.16) of Chapter VII. Forming the product we obtain

$$\Phi(\sigma'_1\sigma''_2|\sigma_1\sigma_2) = \begin{pmatrix} \cos\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} \\ \cos\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}\cos\frac{\alpha''}{2} \\ i\sin\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} \\ i\sin\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}\cos\frac{\alpha''}{2} \end{pmatrix} \quad (2.2.2)$$

And by Feynman's law, the wave function (2.1.2) corresponds to the following wave function in the $\sigma'_1\sigma''_2$ basis:

$$\begin{aligned} \Phi(\sigma'_1\sigma''_2|Y) &= \begin{pmatrix} \cos\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} \\ \cos\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}\cos\frac{\alpha''}{2} \\ i\sin\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} \\ i\sin\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & i\sin\frac{\alpha'}{2}\cos\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}i\sin\frac{\alpha''}{2} & \cos\frac{\alpha'}{2}\cos\frac{\alpha''}{2} \end{pmatrix} \begin{pmatrix} 0 \\ e^{i\alpha/\sqrt{2}} \\ -e^{i\alpha/\sqrt{2}} \\ 0 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} e^{i\alpha} \begin{pmatrix} i\sin\frac{\alpha''-\alpha'}{2} \\ \cos\frac{\alpha''-\alpha'}{2} \\ -\cos\frac{\alpha''-\alpha'}{2} \\ -i\sin\frac{\alpha''-\alpha'}{2} \end{pmatrix} \end{aligned} \quad (2.2.3)$$

Our degrees of belief that $\sigma'_1\sigma''_2 = \frac{1}{2}\frac{1}{2}$, $\frac{1}{2}-\frac{1}{2}$, $-\frac{1}{2}\frac{1}{2}$ or $-\frac{1}{2}-\frac{1}{2}$, under knowledge Y , (i.e. that the (un-measured) system possesses these values under knowledge Y) are therefore

$$\begin{aligned} |\Phi(\frac{1}{2}\frac{1}{2}|Y)|^2 &= \frac{1}{2}(\sin\frac{\alpha''-\alpha'}{2})^2, & |\Phi(\frac{1}{2}-\frac{1}{2}|Y)|^2 &= \frac{1}{2}(\cos\frac{\alpha''-\alpha'}{2})^2, \\ |\Phi(-\frac{1}{2}\frac{1}{2}|Y)|^2 &= \frac{1}{2}(\cos\frac{\alpha''-\alpha'}{2})^2, & |\Phi(-\frac{1}{2}-\frac{1}{2}|Y)|^2 &= \frac{1}{2}(\sin\frac{\alpha''-\alpha'}{2})^2 \end{aligned} \quad (2.2.4)$$

And in particular the result

$$|\Phi(\frac{1}{2}\frac{1}{2}|Y)|^2 = \frac{1}{2}(\sin\frac{\alpha''-\alpha'}{2})^2 \quad (2.2.5)$$

for our degree of belief that the z components of spin of particles 1 and 2 are each $\frac{1}{2}$ in coordinate systems O' and O'' respectively must hold for any angles α' and α'' of the z axes of O' and O'' relative to the original coordinate system O . And this is deemed to be inconsistent with any local-action classical statistical theory claiming (as we do) possessed values of σ'_1 and σ''_2 for all angles α' and α'' .

For suppose, the argument goes, we take three directions a, b and c out from the origin (of our original coordinates O) in the yz plane. Taking the z' axis of O' in one or other of the directions a, b, c and the z'' axis of O'' in one or other of the directions a, b, c , there should (under knowledge Y) be definite (classical) probabilities for the spin components being $\frac{1}{2}$ (or $-\frac{1}{2}$) in each direction. Let $\sigma_1^a, \sigma_1^b, \sigma_1^c$ be the σ_1' spin components of particle 1 with z' in the directions a, b, c respectively, and let $\sigma_2^a, \sigma_2^b, \sigma_2^c$ be the σ_2'' spin components of particle 2 with z'' in the directions a, b, c respectively. Then, thinking still in terms of a statistical hidden-variables theory, we might want to claim that under knowledge Y there is a joint classical probability distribution $p(\sigma_1^a, \sigma_1^b, \sigma_1^c; \sigma_2^a, \sigma_2^b, \sigma_2^c)$ over the values $\sigma_1^a = \pm \frac{1}{2}, \sigma_1^b = \pm \frac{1}{2}, \dots, \sigma_2^c = \pm \frac{1}{2}$, or (more briefly expressed) over the values $\sigma_1^a = \pm, \sigma_1^b = \pm, \dots, \sigma_2^c = \pm$. But assuming (as demonstrated above) full correlation of opposite values of spin components in any one direction, the probabilities $p(\sigma_1^a, \sigma_1^b, \sigma_1^c; \sigma_2^a, \sigma_2^b, \sigma_2^c)$ must be zero when, for example, both σ_1^a and σ_2^a are $+$. Accordingly the non-zero probabilities

$$\begin{aligned}
 p(1) &= p(+++;---) & p(5) &= p(-++;+-- \\
 p(2) &= p(++-;--+) & p(6) &= p(-+-;+ - + \\
 p(3) &= p(+ - +; - + -) & p(7) &= p(- - +; + + -) \\
 p(4) &= p(+ - -; - + +) & p(8) &= p(- - -; + + +)
 \end{aligned}
 \tag{2.2.6}$$

add to 1 and, by the sum rule of classical probability, the probabilities $p(ab)$, $p(bc)$ and $p(ac)$ for spin components of particles 1 and 2 to be $+$ in directions a and b respectively, b and c respectively, and a and c respectively are

$$\begin{aligned}
 p(ab) &= p(3) + p(4) \\
 p(bc) &= p(2) + p(6) \\
 p(ac) &= p(2) + p(4)
 \end{aligned}
 \tag{2.2.7}$$

From which we can deduce the inequality

$$p(ac) \leq p(ab) + p(bc)
 \tag{2.2.8}$$

known as the ‘Bell-Wigner inequality’.

But this inequality is not satisfied by the quantum mechanical degree of belief values in (2.2.5) for all choices of the directions a, b and c . For example taking direction a to be defined by $\alpha' = 60^\circ$ for particle 1 (or $\alpha'' = 60^\circ$ for particle 2), direction b to be defined by $\alpha' = 0^\circ$ for particle 1 (or $\alpha'' = 0^\circ$ for particle 2) and direction c to be defined by $\alpha' = -60^\circ$ for particle 1 (or $\alpha'' = -60^\circ$ for particle 2), we find

$$\begin{aligned}
 |\Phi(ab|Y)|^2 &= |\Phi(\frac{1}{2}|\frac{1}{2}|Y)|^2 = \frac{1}{2}(\sin \frac{\alpha''-\alpha'}{2})^2 = \frac{1}{2}(\sin \frac{0-60^\circ}{2})^2 = \frac{1}{8}, \\
 |\Phi(bc|Y)|^2 &= |\Phi(\frac{1}{2}|\frac{1}{2}|Y)|^2 = \frac{1}{2}(\sin \frac{\alpha''-\alpha'}{2})^2 = \frac{1}{2}(\sin \frac{-60^\circ-0}{2})^2 = \frac{1}{8}, \\
 |\Phi(ac|Y)|^2 &= |\Phi(\frac{1}{2}|\frac{1}{2}|Y)|^2 = \frac{1}{2}(\sin \frac{\alpha''-\alpha'}{2})^2 = \frac{1}{2}(\sin \frac{-60^\circ-60^\circ}{2})^2 = \frac{3}{8},
 \end{aligned} \tag{2.2.9}$$

from which it follows that

$$|\Phi(ac|Y)|^2 > |\Phi(ab|Y)|^2 + |\Phi(bc|Y)|^2 \tag{2.2.10}$$

contradicting (2.2.8).

What are the implications of this contradiction? Does it mean our interpretation of quantum mechanics must be wrong? Well hardly, because we do not consider classical probability to be valid under quantum mechanical conditions. In particular, joint (complex-valued) probability distributions over *incompatible* properties simply do not exist in the new logic of science (see near the ends of sections 2.1 and 3.2 of Chapter I). So there is no probability distribution $\Phi(\sigma_1^a \sigma_1^b \sigma_1^c \sigma_2^a \sigma_2^b \sigma_2^c | Y)$ from which a degree of belief distribution $|\Phi(\sigma_1^a \sigma_1^b \sigma_1^c \sigma_2^a \sigma_2^b \sigma_2^c | Y)|^2$ might be calculated and used in place of the supposed classical probability distribution $p(\sigma_1^a, \sigma_1^b, \sigma_1^c; \sigma_2^a, \sigma_2^b, \sigma_2^c)$ employed above.

However, suppose we take all Bell and Wigner's classical probabilities to be the *actual relative frequencies* in one set of very many trials in which knowledge Y is present in each trial. Then (2.2.7) and (2.2.8) certainly apply as relations between these frequencies. And if we take the calculated degrees of belief in (2.2.5) as giving the *actual relative frequencies* for spin components being both $+\frac{1}{2}$ in O' and O'' (as would appear to be the case from measurements) the contradiction between (2.2.8) and (2.2.10) is back! Back, that is, if the 'probabilities' in (2.2.6) and the degrees of belief in (2.2.9) are the actual frequencies in the set of very many trials. But we avoid the contradiction by simply not claiming that our calculated degrees of belief must necessarily give *actual* frequencies in very many trials. And support for never making this claim is provided by all inequalities of the Bell type.

Of course, we *do* claim to know *expected* frequencies in the set of very many trials. (Expected frequencies are often calculable as shown in section 9 of Chapter II.) And in the above example, the degree of belief values in (2.2.9) are the *expected* frequencies for spin components being both $+\frac{1}{2}$ in O' and O'' for each direction pair ab , bc and ac . We may therefore say that our calculated probability (under knowledge Y) for the proposition $P_1 =$ 'the relative frequency (in the set of very many trials) for the spin components being $+\frac{1}{2}$ in O' and O'' is $\frac{1}{8}$ for direction pair ab ' has modulus 1. But it has an indeterminate phase. And we only *logically expect* P_1 to be true given knowledge Y

of system dynamics in each trial.* Exactly the same remarks apply with regard to proposition P_2 = ‘the relative frequency in the same set of trials for the spin components being $+\frac{1}{2}$ in O' and O'' is $\frac{1}{8}$ for direction pair bc ’ and with regard to proposition P_3 = ‘the relative frequency in the same set of trials for the spin components being $+\frac{1}{2}$ in O' and O'' is $\frac{3}{8}$ for direction pair ac ’.

Now clearly we cannot *logically expect* the truth of the conjunction $P_1P_2P_3$ in the face of (2.2.8) understood, as we are supposing, as an inequality between relative frequencies. We cannot logically expect something that is plainly contradictory! But we do not have to because the propositions P_1 , P_2 and P_3 claim incompatible properties. So while we logically expect the truth of P_1 , P_2 and P_3 *separately*, we should not (by the *law of logical expectation of a conjunction and disjunction* in section 2.2.2 of Chapter I) logically expect the truth of their conjunction. Therefore no contradiction is actually demonstrable.

Does the difference between the (2.2.10) and (2.2.8) lead us to doubt the truth of P_1 , P_2 and P_3 separately since they certainly cannot all be true at once? Well yes, but we had our doubts already, and the difference between the (2.2.10) and (2.2.8) need not alter our *logical expectation* that any *one* of P_1 , P_2 and P_3 is true. And while the truth of P_1 , P_2 or P_3 could be tested (and confirmed) experimentally, the truth or falsity of $P_1P_2P_3$ could of course never be tested experimentally because it would require the measurement of incompatible properties.

The paradoxes arising from other inequalities of the Bell type can be resolved in a way similar to that employed above in connection with the Bell-Wigner inequality. And in each case, the Bell inequality demonstrates our inability to predict actual frequency distributions in repeated trials and the invalidity of taking calculated *expected* frequencies to be *actual* frequencies.

2.3 The validity of the EPR argument

According to the present interpretation of quantum mechanics the argument of Einstein, Podolsky and Rosen is perfectly correct, at least with regard to the system dynamics in section 2.1.

For we clearly see the possibility (at any one time t greater than t_0) of finding, by measurement on particle 1, the spin component σ_2^a of particle 2 in coordinates O'' with z'' in any direction specified by $\alpha'' = \alpha^a$. We simply measure (for example by harmless conditioning as in section 2.1) the spin component σ_1^a of particle 1 in coordinates O' (i.e. with $\alpha' = \alpha^a$) then we know σ_2^a has the value equal and opposite to the known value

* As noted before, we therefore expect the truth of P_1 while allowing that (owing to our limited knowledge) we might be wrong.

of σ_1^a . This measurement can always be performed remotely and has no effect on the spinning motion of particle 2. And under our now pure knowledge regarding particle 2's spin we are free to make an immediate follow up measurement (by harmless conditioning) on particle 2 itself to find its spin component σ_2^b in coordinates O'' specified by $\alpha'' = \alpha^b$. Then we have acquired knowledge of σ_1^a , σ_2^a and σ_2^b at time t . And since all (unmeasured) spin components are constant in time (there being no magnetic field) these values of spin must have been possessed by the particles all the time from t_0 to t . We thus see that the uncertainty principle does not necessarily prevent us from learning the possessed values of incompatible variables *retrospectively* for we have shown here that we can know the values of both σ_2^a and σ_2^b over the time t_0 to t .^{*} Of course in carrying out our measurements we might well have changed the spin components of particle 1 in directions other than a , and we might well have changed the spin components of particle 2 in directions other than b . So with respect to the *future* we cannot simultaneously hold knowledge of spin components of a particle in more than one direction. And 'violation' of the uncertainty principle is only possible with respect to the past. It does not apply to the future, and after all the measurements mentioned, our states of knowledge of the spinning motions of each particle have become logically independent (and therefore uncorrelated), preventing us from repeating a similar set of measurements at a time t' greater than t in order to try to acquire retrospective knowledge also of a further set of incompatible spin component values. So the uncertainty principle is still operating to *limit* the retrospective knowledge we may hold. Nonetheless the fact that we may simultaneously hold knowledge of say σ_2^a and σ_2^b retrospectively supports the belief that spin components (in all directions) are real properties possessed by particles at all times and are not merely products of the process of measurement.

Note that when we hold knowledge of σ_2^a and σ_2^b from times t_0 to t retrospectively (as above), we cannot then claim our knowledge over this period is *pure* even though it was pure once (under knowledge Y before we performed our measurements). Our additional knowledge (concerning spin during the period t_0 to t) renders our previous knowledge *impure*. And it would seem then that a probability distribution (or degree of belief distribution) over the possible values of components of spin σ_2^c in another direction c (between times t_0 and t) is indeterminate. At least, it is not yet clear how it might be calculated.

^{*} Since the first (indirect) measurement (of σ_2^a) left particle 2 untouched, it must also be the case that the spin component σ_1^b that particle 1 had in the b direction before our measurement of σ_1^a must have been equal and opposite to the directly measured value of σ_2^b . So as well as getting to know σ_2^a and σ_2^b from t_0 to t we also get to know σ_1^a and σ_1^b from t_0 to t .

3. Bell's theorem without inequalities

By considering a more complicated system in which *four* spin one-half particles are prepared in a certain way, Greenberger et al [19] have come up with a more direct way of theoretically disproving the EPR notions of locality, reality and completeness. Instead of deriving an (unfulfilled) inequality involving correlation coefficients or probabilities they derive straight contradictions in the predicted relations between spin components of the particles assuming only simple possession of spin components by the particles.

We now show why the present interpretation of quantum mechanics disallows the derivation of contradictions of this kind.

3.1 The system considered by Greenberger et al

Four distinguishable spin one-half particles are present in a space free from any magnetic field. We assume we have pure knowledge Y of their spinning motions represented by the wave function

$$\Phi(\sigma_1\sigma_2\sigma_3\sigma_4|Y) = \frac{1}{\sqrt{2}}(\delta_{\sigma_1\frac{1}{2}}\delta_{\sigma_2\frac{1}{2}}\delta_{\sigma_3-\frac{1}{2}}\delta_{\sigma_4-\frac{1}{2}} - \delta_{\sigma_1-\frac{1}{2}}\delta_{\sigma_2-\frac{1}{2}}\delta_{\sigma_3\frac{1}{2}}\delta_{\sigma_4\frac{1}{2}}) \quad (3.1.1)$$

in the closed sample space $S_{\sigma_1\sigma_2\sigma_3\sigma_4}$ using the z components of spin basis $\sigma_1\sigma_2\sigma_3\sigma_4$ whose natural order is

$$\begin{aligned} \sigma_1\sigma_2\sigma_3\sigma_4 = & \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}, \quad \frac{1}{2}\frac{1}{2}\frac{1}{2}-\frac{1}{2}, \quad \frac{1}{2}\frac{1}{2}-\frac{1}{2}\frac{1}{2}, \quad \frac{1}{2}\frac{1}{2}-\frac{1}{2}-\frac{1}{2}, \\ & \frac{1}{2}-\frac{1}{2}\frac{1}{2}\frac{1}{2}, \quad \frac{1}{2}-\frac{1}{2}\frac{1}{2}-\frac{1}{2}, \quad \frac{1}{2}-\frac{1}{2}-\frac{1}{2}\frac{1}{2}, \quad \frac{1}{2}-\frac{1}{2}-\frac{1}{2}-\frac{1}{2}, \\ & -\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}, \quad -\frac{1}{2}\frac{1}{2}\frac{1}{2}-\frac{1}{2}, \quad -\frac{1}{2}\frac{1}{2}-\frac{1}{2}\frac{1}{2}, \quad -\frac{1}{2}\frac{1}{2}-\frac{1}{2}-\frac{1}{2}, \\ & -\frac{1}{2}-\frac{1}{2}\frac{1}{2}\frac{1}{2}, \quad -\frac{1}{2}-\frac{1}{2}\frac{1}{2}-\frac{1}{2}, \quad -\frac{1}{2}-\frac{1}{2}-\frac{1}{2}\frac{1}{2}, \quad -\frac{1}{2}-\frac{1}{2}-\frac{1}{2}-\frac{1}{2} \end{aligned} \quad (3.1.2)$$

3.2 Calculation of the wave function in more general coordinates

When we refer spin components of particles 1,2,3,4 (of section 3.1) respectively to fixed coordinate systems O_1, O_2, O_3, O_4 of orientations generally different from that of our original coordinate system O (in which (3.1.1) holds), our wave function changes to

$$\Phi(\sigma'_1\sigma'_2\sigma'_3\sigma'_4|Y) = \sum_{\sigma_1\sigma_2\sigma_3\sigma_4} \Phi(\sigma'_1\sigma'_2\sigma'_3\sigma'_4|\sigma_1\sigma_2\sigma_3\sigma_4)\Phi(\sigma_1\sigma_2\sigma_3\sigma_4|Y) \quad (3.2.1)$$

where

$$\Phi(\sigma'_1\sigma'_2\sigma'_3\sigma'_4|\sigma_1\sigma_2\sigma_3\sigma_4) = \Phi(\sigma'_1|\sigma_1)\Phi(\sigma'_2|\sigma_2)\Phi(\sigma'_3|\sigma_3)\Phi(\sigma'_4|\sigma_4) \quad (3.2.2)$$

in which (by (5.16) and the first of (3.6) of Chapter VII) each factor on the RHS has the form

$$\Phi(\sigma'|\sigma) = \begin{pmatrix} \cos \frac{\alpha}{2} e^{i(\beta+\gamma)/2} & i \sin \frac{\alpha}{2} e^{-i(\beta-\gamma)/2} \\ i \sin \frac{\alpha}{2} e^{i(\beta-\gamma)/2} & \cos \frac{\alpha}{2} e^{-i(\beta+\gamma)/2} \end{pmatrix} \quad (3.2.3)$$

α, β and γ being the Euler angles (defined in section 2 of Chapter VII) of coordinate rotation from O . Let the Euler angles for each coordinate system O_1, O_2, O_3 and O_4 be denoted $\alpha_1, \beta_1, \gamma_1; \alpha_2, \beta_2, \gamma_2; \alpha_3, \beta_3, \gamma_3$ and $\alpha_4, \beta_4, \gamma_4$, and let

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \frac{\pi}{2},$$

$$\gamma_1 = \gamma_2 = \gamma_3 = \gamma_4 = 0$$

so that in the matrix notation

$$\Phi(\sigma'_1|\sigma_1) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta_1/2} & ie^{-i\beta_1/2} \\ ie^{i\beta_1/2} & e^{-i\beta_1/2} \end{pmatrix} \quad (3.2.4)$$

and similarly for the other factors on the RHS of (3.2.2).

To develop the corresponding transformation function $\Phi(\sigma'_1\sigma'_2\sigma'_3\sigma'_4|\sigma_1\sigma_2\sigma_3\sigma_4)$ in matrix form we need to work out the Kronecker product

$$\Phi(\sigma'_1|\sigma_1) \otimes \Phi(\sigma'_2|\sigma_2) \otimes \Phi(\sigma'_3|\sigma_3) \otimes \Phi(\sigma'_4|\sigma_4). \quad (3.2.5)$$

The product of the first two terms is

$$\frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta_1/2} & ie^{-i\beta_1/2} \\ ie^{i\beta_1/2} & e^{-i\beta_1/2} \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta_2/2} & ie^{-i\beta_2/2} \\ ie^{i\beta_2/2} & e^{-i\beta_2/2} \end{pmatrix}$$

Working this out and doing the same for the product of the last two factors in (3.2.5) we have

$$\Phi(\sigma'_1\sigma'_2\sigma'_3\sigma'_4|Y) = \frac{1}{4\sqrt{2}} \begin{pmatrix} 0 \\ 2i \\ 2i \\ 0 \\ -2i \\ 0 \\ 0 \\ 2i \\ -2i \\ 0 \\ 0 \\ 2i \\ 0 \\ -2i \\ -2i \\ 0 \end{pmatrix} \quad \text{or} \quad \frac{1}{4\sqrt{2}} \begin{pmatrix} -2i \\ 0 \\ 0 \\ 2i \\ 0 \\ -2i \\ -2i \\ 0 \\ 0 \\ -2i \\ -2i \\ 0 \\ 2i \\ 0 \\ 0 \\ -2i \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix}$$

In the first case the probability is only non-zero for *odd* numbers of negative spin components among the $\sigma'_1\sigma'_2\sigma'_3\sigma'_4$, while in the second case the probability is only non-zero for *even* numbers of negative spin components.

Whenever $\beta_1 + \beta_2 - \beta_3 - \beta_4$ is equal to 0 the probability for an odd number of negative spin components is

$$\Phi\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}-\frac{1}{2} + \frac{1}{2}\frac{1}{2}-\frac{1}{2}\frac{1}{2} + \frac{1}{2}-\frac{1}{2}\frac{1}{2}\frac{1}{2} + \frac{1}{2}-\frac{1}{2}-\frac{1}{2}-\frac{1}{2} + -\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2} + -\frac{1}{2}\frac{1}{2}-\frac{1}{2}-\frac{1}{2} + -\frac{1}{2}-\frac{1}{2}\frac{1}{2}-\frac{1}{2} + -\frac{1}{2}-\frac{1}{2}-\frac{1}{2}\frac{1}{2}\right|Y) = e^{i\varepsilon} \dots (3.3.1)$$

where ε is indeterminate on account of the sum rule.

And whenever $\beta_1 + \beta_2 - \beta_3 - \beta_4$ is equal to π the probability for an even number of negative spin components is

$$\Phi\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2} + \frac{1}{2}\frac{1}{2}-\frac{1}{2}-\frac{1}{2} + \frac{1}{2}-\frac{1}{2}\frac{1}{2}-\frac{1}{2} + \frac{1}{2}-\frac{1}{2}-\frac{1}{2}\frac{1}{2} + -\frac{1}{2}\frac{1}{2}\frac{1}{2}-\frac{1}{2} + -\frac{1}{2}\frac{1}{2}-\frac{1}{2}\frac{1}{2} + -\frac{1}{2}-\frac{1}{2}\frac{1}{2}\frac{1}{2} + -\frac{1}{2}-\frac{1}{2}-\frac{1}{2}-\frac{1}{2}\right|Y) = e^{i\eta} \dots (3.3.2)$$

where η is indeterminate. And this is as much as we can say about ε and η .*

* If the wave function on the RHS of (3.1.1) is realisable only when an indeterminate phase factor is included (as seems likely since the wave function does not go with knowledge of a *basic* property of the

We are thus unable to determine the phases of the probabilities for an odd number of negative spin components, in the first case, or for an even number of negative spin components in the second. But because the moduli of the probabilities are equal to 1, we do *expect* an odd number in the first case and we do *expect* and even number in the second case.

3.4 Greenberger et al's contradiction

Following the argument of Greenberger et al, we define a function $A(\beta_1)$ to be ± 1 according as $\sigma'_1 = \pm \frac{1}{2}$, i.e. according as the spinning motion of particle 1 actually processes the property that its z component of spin in O_1 is $\pm \frac{1}{2}$. Similarly we define functions $B(\beta_2), C(\beta_3)$ and $D(\beta_4)$ in relation to the z components of spin σ'_2, σ'_3 and σ'_4 . Then, from the definition of these functions, and on account of the results (3.3.1) and (3.3.2), we *expect*

$$A(\beta_1)B(\beta_2)C(\beta_3)D(\beta_4) = -1 \quad (3.4.1)$$

whenever $\beta_1 + \beta_2 - \beta_3 - \beta_4 = 0$ and

$$A(\beta_1)B(\beta_2)C(\beta_3)D(\beta_4) = 1 \quad (3.4.2)$$

whenever $\beta_1 + \beta_2 - \beta_3 - \beta_4 = \pi$.

Now we may list the following implications of (3.4.1):

$$\begin{aligned} A(0)B(0)C(0)D(0) &= -1 \\ A(\phi)B(0)C(\phi)D(0) &= -1 \\ A(\phi)B(0)C(0)D(\phi) &= -1 \\ A(2\phi)B(0)C(\phi)D(\phi) &= -1 \end{aligned} \quad (3.4.3)$$

ϕ being an arbitrary angle.

But we must depart from Greenberger et al when they start to reason with results (3.4.3) taken *together*. On the present theory we are blocked from doing this because of the *law of logical expectation of a conjunction and disjunction* (section 2.2.2 of Chapter I) and the fact that the four results in (3.4.3) refer to coordinate systems of different orientation (to different sets of $\beta_1, \beta_2, \beta_3$ and β_4 values) and are therefore claims concerning *incompatible* properties. So we *expect* the truth of the claim represented by any *one* of the equations in (3.4.3), but should not expect the truth of the claim represented by the set of equations taken together.

four spin one-half particle system) then ε in (3.3.1) is (like η in (3.3.2)) indeterminate for more than one reason.

If we disregard the *law of logical expectation of a conjunction and disjunction* we do indeed get contradiction as Greenberger et al show. For the first and second of (3.4.3) give

$$A(\phi)C(\phi) = A(0)C(0)$$

and the first and third give

$$A(\phi)D(\phi) = A(0)D(0)$$

so that

$$\frac{C(\phi)}{D(\phi)} = \frac{C(0)}{D(0)}$$

or since the value of the reciprocal of any one of the functions $A(\beta_1), B(\beta_2), C(\beta_3)$ or $D(\beta_4)$ is the same as its original value (the possible values being only ± 1) we have

$$C(\phi)D(\phi) = C(0)D(0).$$

The last result taken together with the first and last of (3.4.3) gives

$$A(2\phi) = A(0) = \text{const. for all } \phi \quad (3.4.4)$$

which, with $\phi = \frac{\pi}{2}$, contradicts part (ii) of the fourth kinematic property of spin one-half claimed in section 2 of Chapter VII. For the latter implies that $A(0)$ and $A(\pi)$ are equal *and opposite* because they refer to z components of spin in coordinate systems whose z axes point in opposite directions.

A further contradiction arises using (3.4.2) to give

$$A(\theta + \pi)B(0)C(\theta)D(0) = 1$$

for any angle θ . This together with the second of (3.4.3) (with ϕ replaced by θ) gives

$$A(\theta + \pi) = -A(\theta)$$

contradicting (3.4.4) when $\phi = \frac{\pi}{2}$ and $\theta = 0$.

However, as we have said, we cannot arrive at these contradictions because of our *law of logical expectation of a conjunction and disjunction*. Nor, of course, are the predictions (3.4.1) and/or (3.4.2) for different sets of β values together confirmable by measurement, because this would necessitate measurement of incompatible properties which is forbidden by the uncertainty principle. We can however confirm our expectation of the truth represented by (3.4.1) or (3.4.2) for any *one* set of qualifying β values

because, as we have said before, (theoretically valid) expectations under pure states of knowledge seem always to be confirmed by measurement.

But the argument of Greenberger et al serves to show that we definitely cannot claim that expectations (3.4.1) and (3.4.2) (for beta values satisfying $\beta_1 + \beta_2 - \beta_3 - \beta_4 = 0$ and $\beta_1 + \beta_2 - \beta_3 - \beta_4 = \pi$ respectively) reflect *physical laws* controlling the numbers of positive and negative spin components. Although physical laws *can* be the reason for the probabilities of events having moduli 1 and indeterminate phases, they evidently are not the reason in this case. For, if they were, all of (3.4.3) would apply jointly, and contradictions would arise.*

But how can it be that the four properties of the system expressed by equations (3.4.3) cannot all be present (because this would lead to the contradiction (3.4.4)), yet the presence of any one of them seems always to be confirmable by measurement? It seems that we may not conclude, from the fact that any one property is often (and no matter how many times) confirmed by measurement, that it would *always* be so confirmed and so must *always* be present. That is, philosophical ‘induction’ as a process of reasoning is not valid, at least in the present context; for if it were we would arrive again at the contradiction (3.4.4).

Since all four properties (as expressed by equations (3.4.3)) cannot be present, at least one must be absent (on any one occasion) so we might expect at least *occasionally* to find one of the properties absent. Why do we not? Well to account for why we do not we should calculate the probability for finding one of the properties absent. But this we have already done using our new probability theory and the result is zero. So we do not expect to find one of the properties absent and it seems we never do. This may appear amazing but it does not point to a contradiction. No contradiction between theory and experiment can actually be demonstrated. And that is surely all that matters.

4. An alternative to the final part of the first law of potential action

We have claimed, as the final part of the first law of potential action (section 3.2 of Chapter III), that when a particle moves in a scalar potential field its orbital motion during any particular time interval t to $t + dt$ is sometimes influenced by the potential field values at positions that (given our knowledge of its motion) the particle *might* have occupied before time t . This law was generalised to include similar possible influence of any *vector* potential and of any *inter-particle potential* in a system of any number of particles.

* The expectation (with $\beta_1 + \beta_2 - \beta_3 - \beta_4 = 0$) that the number of negative spin components will be odd, and the expectation (with $\beta_1 + \beta_2 - \beta_3 - \beta_4 = \pi$) that the number of negative spin components will be even, amount to expected relations between the spin components. (If, for example $\beta_1 + \beta_2 - \beta_3 - \beta_4 = 0$ and three of the spin components are positive, we *expect* the fourth to be negative.) But these expected relations are different in kind from the relations between the spin components in the system in section 2.1. There (with regard to the two particles present) equal and opposite spin components (in coordinate systems of the same orientation) were a *physical consequence* following acquisition of the pure knowledge Y in section 2.1. Equal and opposite spin components were not just expected, they were considered to be certain.

We also claimed (see for example section 9.2 of Chapter VII) that the spinning motion of a particle during any particular time interval t to $t+dt$ is sometimes influenced by the magnetic field at points the particle might have occupied in the past.

Why did we make this claim about the possible action of passed potentials and magnetic fields? Well, it served to provide a reason why a particle can pass the ‘wrong way’ out of an interferometer when a measurement fails to find the particle in one arm of the interferometer. (See towards the end of section 1.3 of Chapter XII.) And at the same time it did not need to feature in the derivation of the Schrödinger equation because of our previous claim (made in section 3.2 of Chapter I) that, under a *pure* state of knowledge Y in a sample space S covering a time period, knowledge of the potential fields, system potentials functions and magnetic field at times *before* the time covered by S is redundant.

But if the final part of the first law of potential action should seem paradoxical (or unphysical) we can offer another reason a particle is found to leave an interferometer the ‘wrong way’ after null detection in one arm.

In Figure 4.1 we reproduce the Figure in section 1.3 of Chapter XII used in connection with our discussion there about the interferometer in question. We note that

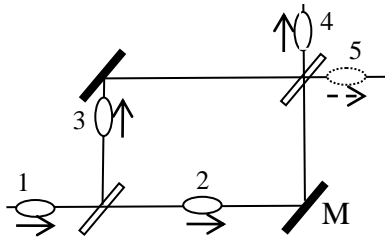


Figure 4.1

the interferometer is such that when no measurement is performed during its operation the similar wave packets 2 and 3 on passing simultaneously through the final half-silvered mirror result in a wave packet 4 (of squared amplitude double that of wave packet 2 or 3) and a wave packet 5 of zero amplitude. This is the result of evolution of the wave function according to the Schrödinger equation. If between times t_1 and t_2 (at which the particle enters and leaves the interferometer) we null detect the particle in the path followed by wave packet 2, packets 4 and 5 have equal amplitude (equal to $1/\sqrt{2}$ times that of 4 previously), while if we carry out no measurement packet 5 is of zero amplitude as we have said.

Instead of claiming that the potential used to null detect the particle (in one arm of the interferometer) causes the particle to sometimes leave in packet 5 rather than always in packet 4, we can claim that the particle is completely *unaffected* by our null measurement potential, and that the fact that the particle is always found to leave in packet 4 (when no measurement is performed) is simply consistent with our *logical expectation* that the particle will be in packet 4 after time t_2 .

This is legitimate because when we work out (using the sum rule) the probability that the particle lies in packet 4 after time t_2 (i.e. the probability that the particle lies in one or other of the volume elements making up the region occupied by packet 4 at a time after time t_2) we get a probability of unit amplitude and *indeterminate* phase. Likewise the probability that the particle lies in one or other of the volume elements making up packet 5 after time t_2 is zero; and zero is also a probability that has an indeterminate phase. So we may just *logically expect* the particle to always leave in packet 4 when no measurement is performed.*

Thus the final part of the first law of potential action may not be needed. But it can be maintained if we wish, and used to account for the particle behaviour in an interferometer when null detection is achieved in one arm. For (as commonly found in classical physics) there is generally more than one way of soundly formulating a physical theory.

* As we have said before logical expectations under pure knowledge are seemingly always borne out by observation, so this approach agrees well enough with our observations.

APPENDIX A. Evaluation of an integral

With the power-one-half function defined by

$$(re^{i\theta})^{1/2} = \sqrt{r}e^{i\frac{\theta}{2}}, \quad -\pi < \theta \leq \pi, \quad r \geq 0$$

(so the cut in the complex plane is taken along the negative x axis) we prove the result

$$\int_{-\infty}^{\infty} e^{i(\alpha(x_2-x_1)^2 + \beta(x_3-x_2)^2 + \gamma(x_2-x_1) + \varepsilon(x_3-x_2))} dx_2 = \left(\frac{i\pi}{\alpha + \beta} \right)^{1/2} e^{i\left(\frac{\alpha\beta}{\alpha+\beta}(x_3-x_1)^2 + \frac{\alpha\varepsilon + \beta\gamma}{\alpha+\beta}(x_3-x_1) - \frac{1}{4} \frac{(\gamma-\varepsilon)^2}{\alpha+\beta}\right)} \quad (\text{A.1})$$

for all real x_1 and x_3 , provided $\alpha + \beta \neq 0$ and

$$\text{Im}(\alpha + \beta) > 0 \quad \text{or} \quad \text{Im}(\alpha) = \text{Im}(\beta) = \text{Im}(\gamma - \varepsilon) = 0. \quad (\text{A.2})$$

Proof:

One or other of conditions (A.2) is clearly necessary for the integral in (A.1) to converge at infinite x_2 (for any real values of x_1 and x_3). Completing the square in x_2 we have that

$$\alpha(x_2 - x_1)^2 + \beta(x_3 - x_2)^2 + \gamma(x_2 - x_1) + \varepsilon(x_3 - x_2) = \frac{\pi}{2}u^2 + c$$

where

$$u = \sqrt{\frac{2}{\pi}} \left((\alpha + \beta)^{1/2} x_2 - \frac{\alpha x_1 + \beta x_3 - \frac{1}{2}(\gamma - \varepsilon)}{(\alpha + \beta)^{1/2}} \right) \quad (\text{A.3})$$

and

$$c = \frac{\alpha\beta}{\alpha + \beta}(x_3 - x_1)^2 + \frac{\alpha\varepsilon + \beta\gamma}{\alpha + \beta}(x_3 - x_1) - \frac{1}{4} \frac{(\gamma - \varepsilon)^2}{\alpha + \beta}. \quad (\text{A.4})$$

Denoting the integral in (A.1) by I we thus have

$$I = J e^{ic}, \quad (\text{A.5})$$

$$J = \int_{-\infty}^{\infty} e^{\frac{i\pi}{2}u^2} dx_2. \quad (\text{A.6})$$

Now, by (A.3), $du = (2(\alpha + \beta)/\pi)^{1/2} dx_2$ so in (A.6) we can replace dx_2 by $(2(\alpha + \beta)/\pi)^{-1/2} du$ and regard J as a contour integral (in the complex u plane) along the contour C given by the locus (A.3) in which x_2 is taken as a real parameter going from $-\infty$ to ∞ . Hence

$$J = (2(\alpha + \beta)/\pi)^{-1/2} \int_C e^{\frac{i\pi}{2}u^2} du. \quad (\text{A.7})$$

Under (A.2), and in the complex u plane, C is either (i) (when $\text{Im}(\alpha + \beta) > 0$) a straight contour of positive slope as x_2 increases or (ii) (when $\alpha + \beta < 0$) a contour along the y axis directed in the positive y direction or (iii) (when $\alpha + \beta > 0$) already a contour along the x axis directed in the positive direction as x_2 increases. In cases (i) and (ii) we can change the contour to one (in the positive direction) along the x axis. This is because $e^{\frac{i\pi}{2}u^2}$ is regular everywhere and on the circular arcs $u = Re^{i\theta}$ where R is constant we have

$$e^{\frac{i\pi}{2}u^2} = e^{\frac{i\pi}{2}R^2(\cos^2\theta - \sin^2\theta)} e^{-\pi R^2 \cos\theta \sin\theta}$$

which tends to zero very rapidly for $R \rightarrow \infty$ when $0 < \theta < \pi/2$ or $\pi < \theta < 3\pi/2$, i.e. on the arcs needed to demonstrate the equivalence of the original contour C and a contour along the x axis. Hence

$$\int_C e^{\frac{i\pi}{2}u^2} du = \int_{-\infty}^{\infty} e^{\frac{i\pi}{2}x^2} dx = (2i)^{1/2}$$

where the value $(2i)^{1/2}$ of the integral follows from 7.3.1, 7.3.2 and 7.3.20 of [21].

Collecting together results we now easily confirm the truth of (A.1) under condition (A.2).

APPENDIX B. Representations of the delta function

Let $f(x)$ be any normal function, bounded and integrable over a real parameter x . Along with or in connection with functions of this kind we use certain representations of the delta function $\delta(x)$ at various places in this monograph. We give here proofs that each of these representations holds true in the sense that

$$\int_{-\infty}^{\infty} f(x) \delta(x) dx = f(0).$$

Representation 1.

We prove first that in order for

$$k\lambda^{-1/2} e^{\frac{i x^2}{\lambda} + i\mu x} = \delta(x) \tag{B.1}$$

i.e. in order for the function $k\lambda^{-1/2} e^{\frac{i x^2}{\lambda} + i\mu x}$ of a real variable x (where k, λ and μ are complex parameters and the power-one-half function is defined as in Appendix A) to equal or represent the delta function $\delta(x)$ (for any complex value of μ) it is necessary that

$$\text{Im}(\lambda) < 0, \tag{B.2}$$

that

$$k = (i\pi)^{-1/2}, \tag{B.3}$$

and that we take the limit

$$\lambda \rightarrow 0. \tag{B.4}$$

Proof:

We require that

$$\int_{-\infty}^{\infty} f(x) k\lambda^{-1/2} e^{\frac{i x^2}{\lambda} + i\mu x} dx = f(0) \tag{B.5}$$

for all normal integrable functions $f(x)$ whose moduli (we suppose) are bounded above.

Note that λ cannot be zero because (B.5) is then undefined. By putting $\lambda = re^{i\theta}$ where $r > 0$ and $-\pi < \theta \leq \pi$, (B.5) becomes

$$\int_{-\infty}^{\infty} f(x) k \frac{1}{\sqrt{r}} e^{-\frac{i\theta}{2}} \exp\left(i \frac{x^2}{r} e^{-i\theta} + i\mu x\right) dx = f(0)$$

or with $x = y\sqrt{r}$

$$\int_{-\infty}^{\infty} f(y\sqrt{r}) k e^{-\frac{i\theta}{2}} \exp(iy^2 e^{-i\theta} + i\mu y\sqrt{r}) dy = f(0). \quad (\text{B.6})$$

This integral exists only if $\text{Im}(e^{-i\theta}) > 0$ (or $-\pi < \theta < 0$) and this confirms the need for (B.2). Now (B.6) can only be satisfied by letting $r \rightarrow 0$ so that the LHS of (B.6) becomes $f(0)$ times a constant and this confirms the need for (B.4). Finally in order that the constant is equal to 1 we need

$$\int_{-\infty}^{\infty} \exp(iy^2 e^{-i\theta}) dy = \frac{1}{k} e^{\frac{i\theta}{2}}. \quad (\text{B.7})$$

The integral here is a special case of the integral in (A.1) of Appendix A and therefore equals $(i\pi)^{1/2} e^{i\theta/2}$ and so we confirm the need for (B.3). QED.

Corollary1:

If (B.1) is required only for real μ , (B.2) can be relaxed to

$$\text{Im}(\lambda) \leq 0, \quad (\text{B.8})$$

This is because with μ real the integral in (B.6) now exists when $\theta = 0$ and, under (B.3), (B.7) still holds when $\theta = 0$.

Corollary2:

If (B.1) is to hold for $\text{Im}(\lambda) = 0$ and $\lambda \rightarrow 0$, then μ must be restricted to real values, i.e.

$$\text{Im}(\mu) = 0. \quad (\text{B.9})$$

And (B.3) is still the necessary value for the constant k .

Representation 2.

We show that for real α

$$\delta(x) = \frac{1}{\pi} \lim_{\alpha \rightarrow \infty} \frac{\sin x\alpha}{x}. \quad (\text{B.10})$$

Proof:

$$\lim_{\alpha \rightarrow \infty} \int_{-\infty}^{\infty} \frac{\sin x\alpha}{x} f(x) dx$$

can be evaluated by putting $x\alpha = t$ transforming it to

$$\lim_{\alpha \rightarrow \infty} \int_{-\infty}^{\infty} \frac{\sin t}{t} f\left(\frac{t}{\alpha}\right) dt = f(0) \int_{-\infty}^{\infty} \frac{\sin t}{t} dt = \pi f(0).$$

(See 4.3.141, p78 of [21].) QED.

Representation 3.

Similarly we show that for real α

$$\delta(x) = \frac{1}{\pi} \lim_{\alpha \rightarrow \infty} \frac{\sin^2 x\alpha}{x^2 \alpha}. \quad (\text{B.11})$$

Proof:

$$\lim_{\alpha \rightarrow \infty} \int_{-\infty}^{\infty} \frac{\sin^2 x\alpha}{x^2 \alpha} f(x) dx$$

can be evaluated by putting $x\alpha = t$ transforming it to

$$\lim_{\alpha \rightarrow \infty} \int_{-\infty}^{\infty} \frac{\sin^2 t}{t^2} f\left(\frac{t}{\alpha}\right) dt = f(0) \int_{-\infty}^{\infty} \frac{\sin^2 t}{t^2} dt.$$

Here

$$\int_{-\infty}^{\infty} \frac{\sin^2 t}{t^2} dt = \int_{-\infty}^{\infty} \frac{1}{2} \frac{(1 - \cos 2t)}{t^2} dt = \int_0^{\infty} \frac{1 - \cos 2t}{t^2} dt = \lim_{t \rightarrow 0} \left[-t^{-1} - \int \frac{\cos 2t}{t^2} dt \right]_t^{\infty}.$$

Putting $2t = z$ the integral in the square brackets becomes (using integration by parts)

$$\int \frac{\cos 2t}{t^2} dt = 2 \int \frac{\cos z}{z^2} dz = 2 \left[-\frac{\cos z}{z} - \int \frac{\sin z}{z} dz \right].$$

And thus we find

$$\int_{-\infty}^{\infty} \frac{\sin^2 t}{t^2} dt = \lim_{t \rightarrow 0} \left[-\frac{2}{z} + 2 \frac{\cos z}{z} + 2 \int \frac{\sin z}{z} dz \right]_t^{\infty} = 2 \int_0^{\infty} \frac{\sin z}{z} dz = \pi.$$

(See 4.3.141, p78 of [21].) QED.

Representation 4.

We have

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ixt} dt = \delta(x)$$

in the sense that the LHS is

$$\lim_{L \rightarrow \infty} \frac{1}{2\pi} \frac{e^{ixt}}{ix} \Big|_{t=-L}^{t=L} = \lim_{L \rightarrow \infty} \frac{1}{\pi x} \frac{e^{ixL} - e^{-ixL}}{2i} = \lim_{L \rightarrow \infty} \frac{1}{\pi} \frac{\sin xL}{x}$$

which by (B.10) is $\delta(x)$. QED.

APPENDIX C. The electromagnetic field in non-relativistic quantum mechanics.

Quantum mechanical charge and system potentials

A quantum mechanical particle may carry a charge. And this acts as a source of electric potential much in the same way as a charged particle does in classical electromagnetism. But (unlike in classical electromagnetism) a quantum mechanical charged particle in motion does not produce a magnetic field or an electromagnetic vector potential.*

Charge is responsible for (electromagnetic) quantum mechanical inter-particle (scalar) potentials and for quantum mechanical particle (scalar and vector) potentials in any external electromagnetic field produced by macroscopic sources. Let the charges carried by the N particles of a quantum mechanical system be q_i^\dagger , $i = 1, \dots, N$ and let the particle coordinates in a fixed coordinate system O be \mathbf{r}_i , $i = 1, \dots, N$. With respect to O , if the electric potential of the external electric field is $\phi(\mathbf{r}, t)$, then in the formula for the system potential in (2.1) of Chapter V, we will have (in the absence of other (i.e. non-electromagnetic) potentials)

$$V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) = \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (\text{C.1})$$

and

$$V_i(\mathbf{r}_i, t) = q_i \phi(\mathbf{r}_i, t). \quad (\text{C.2})$$

And if the external electromagnetic field includes a vector potential $\mathbf{A}(\mathbf{r}, t)^\ddagger$ each particle experiences a quantum mechanical vector potential $\mathbf{A}_i(\mathbf{r}_i, t)$ given by

$$\mathbf{A}_i(\mathbf{r}_i, t) = q_i \mathbf{A}(\mathbf{r}_i, t) / c \quad (\text{C.3})$$

c being the velocity of light in vacuo.

* By supposing charged particles in quantum mechanics produce no electromagnetic vector potentials or magnetic fields we make impossible the quantum mechanical modelling of the macroscopic sources of such fields. This is a shortcoming of non-relativistic quantum mechanics that can be overcome only after its relativistic generalisation.

† Unless otherwise stated, we employ (for electromagnetic quantities) Gaussian units as in [12] and [15].

‡ In the main text we denote the electromagnetic vector potential by \mathbf{A}_{em} (rather than \mathbf{A}) to distinguish it from the quantum mechanical vector potential \mathbf{A} . But in this Appendix it is appropriate to use \mathbf{A} rather (than \mathbf{A}_{em}) in keeping with the usual notation in electromagnetic theory.

The external electromagnetic field equations

In non-relativistic quantum mechanics external electromagnetic fields are the product of macroscopic matter (forming macroscopic sources). The essential properties of that matter and the electromagnetic fields it produces are (like the kinematic properties of coordinate systems) not subject to the uncertainty principle.

For use in connection with non-relativistic quantum mechanics we state the following three laws governing the sources and their fields relative to any rest frame O in which position is denoted by \mathbf{r} and time by t .

Law 1. There are distributed and effectively continuous macroscopic charges and currents with densities $\rho(\mathbf{r},t)$ and $\mathbf{J}(\mathbf{r},t)$ respectively and we suppose (in our modelling) that these densities are under our control. We consider the charges and currents to be carried in (generally moving) rigid bodies that have themselves no effect on the electromagnetic fields. We assume the motion of these bodies is also under our control. The source densities are assumed to satisfy conservation equations according to which, at any one time t

$$\left. \begin{aligned} \int \rho d\tau &= Q \\ \nabla \cdot \mathbf{J} &= 0 \\ \int \mathbf{J} \cdot d\mathbf{S} &= 0 \end{aligned} \right\} \quad (\text{C.4})$$

where Q is a constant (independent of t), the first (volume) integral is over all space and the second (surface) integral may be over any closed surface or any surface dividing space into two parts.

Law 2. If the body carrying charge is supposed to move with an extra uniform velocity \mathbf{v} , and is coincident with its previous position at time $t=0$, then $\rho(\mathbf{r},t)$ changes to $\rho(\mathbf{r}-\mathbf{v}t,t)$. If the body carrying current likewise moves with an extra velocity \mathbf{v} then $\mathbf{J}(\mathbf{r},t)$ changes to $\mathbf{J}(\mathbf{r}-\mathbf{v}t,t)$ and an *additional charge source* of density*

$$\mathbf{v} \cdot \mathbf{J}(\mathbf{r}-\mathbf{v}t,t)/c^2$$

* This additional charge source is in fact a relativistic effect. It arises because of the difference in Lorentz contraction of the spacing between the positive and negative charge carriers (constituting the current source) on account of those charges moving at different speeds (see pp. 333-334 of [13]). This is one of the reasons a relativistic quantum theory is needed to model the macroscopic sources.

arises within the body.*

Law 3. The sources produce a scalar electric potential field $\phi(\mathbf{r}, t)$ and a vector magnetic potential field $\mathbf{A}(\mathbf{r}, t)$ in O according to the rules[†]

$$\phi = \int \frac{\rho}{r} d\tau, \quad (\text{C.5})$$

$$\mathbf{A} = \frac{1}{c} \int \frac{\mathbf{J}}{r} d\tau. \quad (\text{C.6})$$

which give the potentials ϕ and \mathbf{A} at any point P in fixed space and at any moment in time. In (C.5) and (C.6) ρ and \mathbf{J} are the charge and current densities at the time in question and r is the distance from P to the general spatial volume element $d\tau$ in the integrals.

It follows from the relations ((C.2) and (C.3)) between the electromagnetic potentials and the quantum mechanical potentials that when a particle of the quantum mechanical system carries a charge q , has become free of the influence of the other particles of the system and moves in the classical limit in the external electromagnetic field specified by potentials fields ϕ and \mathbf{A} , it is expected to do so as if it obeyed Newton's second law of motion and experienced a force \mathbf{F} given by[‡]

$$\mathbf{F} = q\left(-\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} - \nabla\phi + \frac{1}{c} \mathbf{u} \times (\nabla \times \mathbf{A})\right) \quad (\text{C.7})$$

where \mathbf{u} is the particle velocity relative to O and ϕ and \mathbf{A} are the electric and magnetic potentials in the vicinity of the point occupied by the particle at the time in question, $\partial \mathbf{A} / \partial t$ denoting the local rate of change of \mathbf{A} (not the rate of change of \mathbf{A} following the particle).

Galilean invariance of the external field equations

We can demonstrate that the external field equations are Galilean invariant.

The transformation equations under a velocity boost of coordinates are

$$\mathbf{u} = \mathbf{u}' + \mathbf{v} \quad (\text{C.8})$$

$$\mathbf{F} = \mathbf{F}' \quad (\text{C.9})$$

* The first condition in (C.4) is not violated by the appearance of this additional charge density because

$\int \mathbf{v} \cdot \mathbf{J}(\mathbf{r} - \mathbf{v}t, t) d\tau$ can be expressed as the sum of fluxes of \mathbf{J} through plane surfaces perpendicular to the vector \mathbf{v} and by the last of (C.4) each of these fluxes is zero.

[†] These are the same as the well known formulae of the quasi-static and quasi-stationary potential fields of classical electromagnetism.

[‡] see near the end of section 1 of Chapter III

$$q_i = q'_i \quad (\text{C.10})$$

$$\mathbf{J} = \mathbf{J}' \quad (\text{C.11})$$

$$\mathbf{A} = \mathbf{A}' \quad (\text{C.12})$$

$$\rho = \rho' + \mathbf{v} \cdot \mathbf{J}' / c^2 \quad (\text{C.13})$$

$$\phi = \phi' + \frac{1}{c} \mathbf{v} \cdot \mathbf{A}' \quad (\text{C.14})$$

where (C.8)-(C.10) relate to (C.7). And the same external field *Laws* 1,2 and 3 above (as well as the force rule (C.7)) apply under this transformation, which is from coordinate frame O' to coordinate frame O , where O' moves with constant velocity \mathbf{v} , the origin of O' being at $\mathbf{v}t$ at time t . The un-primed variables on the LHS of (C.8)-(C.14) refer to position \mathbf{r} in O at time t and the primed variables on the RHS to position \mathbf{r}' in O' at time t with $\mathbf{r}' = \mathbf{r} - \mathbf{v}t$.

Now (C.8), (C.10) and (C.11) are evidently true from classical kinematics and the assumed invariant character of particle charges and current sources. (C.12) accords with (C.6) and (C.11). (C.13) follows from *Law* 2 on account of the fact that observers O and O' differ in regard to what they consider to be fixed space - so if O' considers the body carrying the current density to be at rest, O considers it to be in motion with velocity \mathbf{v} , and in general O considers it to have an *additional* velocity \mathbf{v} . Observers O and O' therefore differ with regard to the distribution of charge density and therefore to the value of the electric potential which O finds by applying (C.5) and O' finds by applying the first of the potential formulae

$$\phi' = \int \frac{\rho'}{r} d\tau, \quad \mathbf{A}' = \frac{1}{c} \int \frac{\mathbf{J}'}{r} d\tau \quad (\text{C.15})$$

in O' . Using (C.15) with (C.13) we have

$$\phi = \int \frac{\rho}{r} d\tau = \int \frac{\rho' + \mathbf{v} \cdot \mathbf{J}' / c^2}{r} d\tau = \phi' + \frac{1}{c} \mathbf{v} \cdot \mathbf{A}'$$

agreeing with the transformation formula (C.14).

Finally the invariance, as in (C.9), of the force (C.7) is shown as follows. First note that by (C.12)

$$\frac{\partial \mathbf{A}}{\partial t} = \frac{\partial}{\partial t} \mathbf{A}(\mathbf{r}, t) = \frac{\partial}{\partial t} \mathbf{A}'(\mathbf{r} - \mathbf{v}t, t) = \frac{\partial \mathbf{A}'}{\partial t} - (\mathbf{v} \cdot \nabla) \mathbf{A}'$$

and, by (C.14), $\nabla \phi = \nabla \phi' + \frac{1}{c} \nabla(\mathbf{v} \cdot \mathbf{A}')$. These give

$$-\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} - \nabla \phi + \frac{1}{c} \mathbf{u} \times (\nabla \times \mathbf{A}) = -\frac{1}{c} \left(\frac{\partial \mathbf{A}'}{\partial t} - (\mathbf{v} \cdot \nabla) \mathbf{A}' \right) - \nabla \phi' - \frac{1}{c} \nabla(\mathbf{v} \cdot \mathbf{A}') + \frac{1}{c} (\mathbf{u}' + \mathbf{v}) \times (\nabla \times \mathbf{A}')$$

and since $\nabla(\mathbf{v}\cdot\mathbf{A}') = (\mathbf{v}\cdot\nabla)\mathbf{A}' + \mathbf{v}\times(\nabla\times\mathbf{A}')$ on account of \mathbf{v} being constant, this becomes

$$-\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} - \nabla\phi + \frac{1}{c}\mathbf{u}\times(\nabla\times\mathbf{A}) = -\frac{1}{c}\frac{\partial\mathbf{A}'}{\partial t} - \nabla\phi' + \frac{1}{c}\mathbf{u}'\times(\nabla\times\mathbf{A}')$$

in agreement with (C.9) under (C.10).

The external electric and magnetic fields and Maxwell's equations

We can define the electric field \mathbf{E} and magnetic field \mathbf{H} as*

$$\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} - \nabla\phi. \quad (\text{C.16})$$

$$\mathbf{H} = \nabla\times\mathbf{A} \quad (\text{C.17})$$

From (C.5) and (C.6) and the fact that $\nabla\cdot\mathbf{J} = 0$ it follows that

$$-\nabla^2\phi = 4\pi\rho, \quad (\text{C.18})$$

$$-\nabla^2\mathbf{A} = \frac{4\pi}{c}\mathbf{J}, \quad (\text{C.19})$$

$$\nabla\cdot\mathbf{A} = 0, \quad (\text{C.20})$$

and therefore that

$$\nabla\cdot\mathbf{E} = 4\pi\rho \quad (\text{C.21})$$

$$\nabla\cdot\mathbf{H} = 0 \quad (\text{C.22})$$

$$\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{H}}{\partial t} \quad (\text{C.23})$$

$$\nabla\times\mathbf{H} = \frac{4\pi}{c}\mathbf{J} \quad (\text{C.24})$$

which are the quasi-static/quasi-stationary form of Maxwell's equations.

The effective force (C.7) on a quantum mechanical particle of charge q in the classical limit becomes

$$\mathbf{F} = q\left(\mathbf{E} + \frac{1}{c}\mathbf{u}\times\mathbf{H}\right) \quad (\text{C.25})$$

which is the Lorentz law.

The transformation equations for the electric and magnetic fields under a velocity boost of coordinates are, by (C.16), (C.17), (C.12) and (C.14)

* In the units employed we have also (in the assumed vacuum) $\mathbf{B} = \mathbf{H}$ and $\mathbf{D} = \mathbf{E}$.

$$\mathbf{E} = \mathbf{E}' - \frac{1}{c} \mathbf{v} \times \mathbf{H}' \quad (\text{C.26})$$

$$\mathbf{H} = \mathbf{H}' \quad (\text{C.27})$$

Orders of magnitude

Using a large enough steady current density source we can produce a strong constant magnetic potential field to interact with a quantum mechanical system. Also, using a large enough charge density source we can produce a strong static electric potential field to interact with a quantum mechanical system, and by varying the charge or current sources or moving the bodies carrying them, we can produce time varying fields, for example alternating fields.*

The limits of applicability of the quasi-static/quasi-stationary field equations adopted can be got from comparison with the full Maxwell equations with charge and current sources and the full Lorentz transformation equations. In MKS units the full Maxwell equations are (see for example [13])

$$\nabla \cdot \mathbf{E} = \rho / \epsilon_0 \quad (\text{C.28})$$

$$\nabla \cdot \mathbf{B} = 0 \quad (\text{C.29})$$

$$\nabla \times \mathbf{E} = -\partial \mathbf{B} / \partial t \quad (\text{C.30})$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \epsilon_0 \mu_0 \partial \mathbf{E} / \partial t \quad (\text{C.31})$$

where $\mathbf{B} = \mu_0 \mathbf{H}$ and the (almost) full Lorentz transformation equations are

$$\mathbf{E} = \mathbf{E}' - \mathbf{v} \times \mathbf{B}' \quad (\text{C.32})$$

$$\mathbf{B} = \mathbf{B}' + \mathbf{v} \times \mathbf{E}' / c^2 \quad (\text{C.33})$$

$$\rho = \rho' + \mathbf{v} \cdot \mathbf{J}' / c^2 \quad (\text{C.34})$$

$$\mathbf{J} = \mathbf{J}' + \rho' \mathbf{v} \quad (\text{C.35})$$

in which only the factor $\gamma (= \sqrt{1 - v^2/c^2})$ has been simplified to 1 in keeping with our non-relativistic treatment.

In the quasi-static/quasi-stationary approximation we are neglecting the last terms in (C.31), (C.33) and (C.35). To see how this is reasonable, suppose that within a cubical body of dimensions $1\text{m} \times 1\text{m} \times 1\text{m}$ (i.e. one cubic meter) we have source densities ρ and \mathbf{J} capable of producing, in or near to the body, electric fields of order 1kVm^{-1} and magnetic flux densities of order 1T . Then by (C.28) and (C.31)

* Modelling of the scattering of electromagnetic waves by quantum systems is not possible because we are assuming that quantum mechanical particles produce no magnetic fields and we are neglecting the displacement current term in Maxwell's equations. Such modelling can anyway only properly be handled in relativistic quantum mechanics.

$$\rho \approx 10^3 \epsilon_0 \text{ Cm}^{-3}$$

$$J \approx 1/\mu_0 \text{ Am}^{-2}.$$

Then in (C.35), (C.33) and (C.31), if f is the typical frequency of variation of \mathbf{E} (or \mathbf{B}) we have (putting $c \approx 3 \times 10^8 \text{ ms}^{-1}$)

$$\frac{\rho' v}{J'} \approx \frac{1}{3} \frac{v}{c} \times 10^{-5}, \quad \frac{v \times E'/c^2}{B'} \approx \frac{1}{3} \frac{v}{c} \times 10^{-5},$$

$$\frac{\mu_0 \epsilon_0 \dot{E}}{\mu_0 J} \approx f \times 10^{-14}.$$

The first two are clearly very small compared to 1 on account of our assumption that $v \ll c$. The third is small compared to 1 up to radio frequencies at which the corresponding wavelength of electromagnetic waves is (as required) still large compared with the dimensions of the source body (i.e. $\gg 1 \text{ m}$).

On the other hand, in (C.34), (C.32) and (C.30) we have

$$\frac{v \cdot \mathbf{J}'/c^2}{\rho'} \approx v \times 10^{-3}, \quad \frac{v \times \mathbf{B}'}{E'} \approx v \times 10^{-3}$$

$$\frac{\partial \mathbf{B}/\partial t}{E/l} \approx f \times 10^{-3}$$

where l is a typical dimension of the source distributions. None of these ratios is necessarily negligible.

The second law of potential action

Relative to inertial frame O considered to be at rest, let $\phi(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ be electromagnetic potential fields generated by (macroscopic) sources. These give rise, by (C.2) and (C.3), to quantum mechanical external potentials

$$V_i(\mathbf{r}_i) = q_i \phi(\mathbf{r}_i, t) \tag{C.36}$$

$$\mathbf{A}_i(\mathbf{r}_i, t) = q_i \mathbf{A}(\mathbf{r}_i, t)/c \tag{C.37}$$

on the i^{th} particle of a quantum mechanical system. We have postulated in *Law 2* above that if the bodies carrying the sources are given a velocity boost \mathbf{v} and have the same positions in space at time $t=0$, then the sources change from $\rho(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$ to $\rho(\mathbf{r} - \mathbf{v}t, t) + \mathbf{v} \cdot \mathbf{J}(\mathbf{r} - \mathbf{v}t, t)/c^2$ and $\mathbf{J}(\mathbf{r} - \mathbf{v}t, t)$. By (C.5) and (C.6) the potential fields thus change to $\phi(\mathbf{r} - \mathbf{v}t, t) + \mathbf{v} \cdot \mathbf{A}(\mathbf{r} - \mathbf{v}t, t)/c$ and $\mathbf{A}(\mathbf{r} - \mathbf{v}t, t)$. Accordingly the quantum mechanical potentials (C.36) and (C.37) change from $V_i(\mathbf{r}_i)$ and $\mathbf{A}_i(\mathbf{r}_i, t)$ to

$V_i(\mathbf{r}_i - \mathbf{v}t) + \mathbf{v} \cdot \mathbf{A}_i(\mathbf{r}_i - \mathbf{v}t, t)$ and $\mathbf{A}_i(\mathbf{r} - \mathbf{v}t_i, t)$ in agreement with the second law of potential action (section 3.2 of Chapter III).

So when the external potentials are electromagnetic in origin the second law of potential action (section 3.2 of Chapter III) is a consequence of the electromagnetic field equations in their quasi-static/quasi-stationary form.

The internal electromagnetic field equations

In any quantum mechanical system containing charged particles (e.g. a hydrogen atom) there is an internal (electric) potential field. The sources of this field are the charged particles themselves. If the i^{th} particle has charge q_i it causes an internal electric potential at position \mathbf{r} given, at any time t , by

$$\phi_i = \frac{q_i}{|\mathbf{r} - \mathbf{r}_i|}$$

where \mathbf{r}_i is the position of the i^{th} particle at time t . It is this potential that gives rise to the inter-particle potential V_{ij} in (C.1). Since the value of \mathbf{r}_i is generally unknown and subject to the uncertainty principle, so is the value of ϕ_i at any given point \mathbf{r} .

In non-relativistic quantum mechanics the internal (electric) potential can be thought of as quasi-static. The charged particles of a quantum mechanical system are moving at speeds small compared to the speed of light and, as we have said, they are assumed not to generate electromagnetic vector potential fields (even weakly).

When considering the *total* electromagnetic field we should of course include the internal electric potential field along with any external electromagnetic potentials that may be present. Accordingly the total electromagnetic scalar and vector potentials at any point P and any time t are given by

$$\phi = \int \frac{\rho}{r} d\tau + \sum_i \frac{q_i}{|\mathbf{r} - \mathbf{r}_i|}, \quad (\text{C.38})$$

$$\mathbf{A} = \frac{1}{c} \int \frac{\mathbf{J}}{r} d\tau. \quad (\text{C.39})$$

in place of (C.5) and (C.6). Here \mathbf{r} is the position coordinate of P and ρ, \mathbf{J} and r have of course the same meanings as they have in (C.5) and (C.6), i.e. r is the distance from P to the general volume element $d\tau$ and, ρ and \mathbf{J} are the charge and current densities of the macroscopic sources.

We note that since the \mathbf{r}_i may be non-differentiable functions of the time, $\partial\phi/\partial t$ is now generally non-existent. But this is of no consequence because $\partial\phi/\partial t$ does not feature in essential equations. The *spatial* derivatives, i.e. $\nabla\phi$, still exist (except at the positions of the particles themselves). And so, therefore, do the electric and magnetic fields (as defined in (C.16)-(C.17) with ϕ now given by (C.38)). The Galilean

transformation equations (C.11)-C.14) remain valid, i.e. they apply to the total electromagnetic fields. And so do the quasi-static/quasi-stationary Maxwell's equations (C.16)-(C.24) with ρ now replaced by

$$\rho + \sum_i q_i \delta(\mathbf{r} - \mathbf{r}_i).$$

Note on the relativistic modelling of macroscopic electromagnetic field sources

In the introductory paragraphs of Chapter XIII we claimed that a macroscopic source (set up to produce an external potential field of any kind to interact with a quantum mechanical system) may penetrate that system without affecting it directly. Only the field produced by the overall source affects the system.

To show this claim is reasonable we briefly consider here the relativistic modelling* of the macroscopic charge and current densities sources $\rho(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$ considered in this Appendix. We consider only the case of time independent and uniform ρ and \mathbf{J} in the region R between two fixed parallel planes the direction of \mathbf{J} being parallel to the planes. We model these by supposing they arise from a swarm of charged quantum mechanical particles of very large mass half of which carry charge q_1 and half of which carry charge q_2 . Being of very large mass we may assume the particles are at rest or moving classically in uniform motions. We suppose the particles of a common charge (q_1 or q_2) are distributed uniformly in R , the particles of charge q_1 are all at rest, and those of charge q_2 all move with a uniform velocity u (with $u^2/c^2 \ll 1$) in the direction of the required current density. We take the limit as the number of particles tends to infinity, and the charges tend to zero, while q_1/q_2 , u and the average charge density (of particles of either charge) stay constant.

Let P be a point lying somewhere between the particles. By the laws of electrodynamics in special relativity, the scalar electric potential ϕ at P due to the nearest particle (or to a fixed number of neighbouring particles) is of order q/r (and the electric field E is of order q/r^2) where q is either q_1 or q_2 and r is the distance between P and the nearest particle (the same order as the distance between neighbouring particles). In the limit we are taking, r tends to zero and in order for the average charge density (of particles of either charge) to stay constant it is necessary that $q \sim r^3$. Therefore in this limit both ϕ and E generally tend to zero, the only exception occurring when P remains within a distance δ of the nearest particle where q/δ (or q/δ^2 in the case of the electric field) stays constant during the limiting process. That requires $\delta \sim r^3$ (or $\delta \sim r^{3/2}$ in the case of the electric field). The fraction of the volume of space in R where this is true is δ^3/r^3 which is of order r^6 (or $r^{3/2}$ in the case of the electric field). Therefore in the limit we may say the electric potential ϕ (and the associated electric

* The modelling has to be relativistic. See first footnote in the earlier section headed '*The external electromagnetic field equations*'.

field) at any point P in R is *almost always* zero. As a result the total electric potential (and the total electric field) at any point P in R may be said to be no way due to the neighbouring particles and to result only from the accumulative effect of all the particles of the source.

Exactly similar considerations apply to the magnetic (vector) potential field and the magnetic field produced by the moving particles making up the electromagnetic source in R. At any point P in R these fields too are almost never due to particles close to P and result only from the accumulative effect of all the particles of the source.

Now suppose we place in R a quantum mechanical system of particles, say a hydrogen atom, composed of two particles, an electron and a proton (modelled as material points of zero size). Each of these particles will almost always lie in the space between particles of the source and so will not be affected by the closest particles of the source but only by the electromagnetic field arising from the source particles as a whole. We have no need to impose zero probability for the electron (or the proton) to occupy the same point in space as a particle of the source. For in section 3.7 of Chapter III we have claimed that any number of particles may occupy the same volume element of space with non-zero probability regardless of their kind or their spin components. Therefore even when a quantum mechanical system lies within region R the quantum mechanical theory of its motion can proceed on the basis that only the electromagnetic fields produced by the sources $\rho(\mathbf{r},t)$ and $\mathbf{J}(\mathbf{r},t)$ have an effect on the motion and there is no direct effect from the sources themselves.

Supposing R is $\approx 1\text{m}$ wide, then to produce electric fields $\approx 1\text{kVm}^{-1}$ we need a charge density $\approx 10^{-3}\epsilon_0\text{Cm}^{-3}$ (see section ‘Orders of magnitude’ above). That is we need $n_1q_1 + n_2q_2 \approx 10^{-3}\epsilon_0\text{Cm}^{-3}$ where n_1 and n_2 are the number of particles of charge q_1 and q_2 respectively per unit volume. (As we have said we take $n_1 = n_2$.) We have seen (in section ‘Orders of magnitude’ above) that a velocity u (with $u^2/c^2 \ll 1$) given to the charge density n_2q_2 produces only a negligible current density n_2q_2u if n_2q_2 is of order $10^{-3}\epsilon_0\text{Cm}^{-3}$. Therefore we need (in our model of electromagnetic sources) to take $n_2q_2 \gg 10^{-3}\epsilon_0\text{Cm}^{-3}$ in order that \mathbf{J} can be large enough to produce magnetic fields of order 1T. This can be achieved (while maintaining $n_1q_1 + n_2q_2 \approx 10^{-3}\epsilon_0\text{Cm}^{-3}$) only by taking n_1q_1 and n_2q_2 large in absolute value but opposite in sign (so n_1q_1 and n_2q_2 are nearly equal and opposite).*

If the system of source particles (of charges q_1 and q_2) is given a uniform velocity boost in the direction of the current density, charges q_1 also produce a current density and the net current density becomes $\mathbf{J} = n_1q_1\mathbf{u}_1 + n_2q_2\mathbf{u}_2$ where \mathbf{u}_1 and \mathbf{u}_2 are the net velocities of the particles of charge q_1 and q_2 respectively. The Lorentz contraction of the spaces between particles of either charge is quite negligible here because we assume still that the velocities of the particles are small compared to the speed of light

* This is of course the actual situation in a current carrying conductor where the negative charge density of the free electrons is very large but is cancelled out by the (also very large but positive) combined charge density of the nuclei and bound electrons of the metal atoms.

(i.e. that $u_1^2/c^2 \ll 1$ and $u_2^2/c^2 \ll 1$) and the terms $n_1q_1u_1$ and $n_2q_2u_2$ in the expression for J are not nearly cancelling.

However when it comes to the value of the charge density $n_1q_1 + n_2q_2$, this is affected by the Lorentz contraction. Here the terms n_1q_1 and n_2q_2 do nearly cancel and we need to consider more exactly the values of n_1 and n_2 , and how they change with velocity. Let n_1 and n_2 be the number densities when $u_1 = u_2 = 0$. Let the particles start with velocities u_1 and u_2 (both $\ll c$). Then the Lorentz contraction changes n_1 to $n_1(1 + \frac{u_1^2}{2c^2})$ and n_2 to $n_2(1 + \frac{u_2^2}{2c^2})$ (neglecting higher order correction terms) and the net charge density becomes $n_1(1 + \frac{u_1^2}{2c^2})q_1 + n_2(1 + \frac{u_2^2}{2c^2})q_2$. If a boost v is applied, the Lorentz contraction increases the number densities to $n_1(1 + \frac{(u_1+v)^2}{2c^2})$ and $n_2(1 + \frac{(u_2+v)^2}{2c^2})$, so the net charge density grows by $n_1(1 + \frac{(u_1+v)^2}{2c^2})q_1 + n_2(1 + \frac{(u_2+v)^2}{2c^2})q_2 - n_1(1 + \frac{u_1^2}{2c^2})q_1 - n_2(1 + \frac{u_2^2}{2c^2})q_2$ or by $n_1 \frac{u_1v}{c^2} q_1 + n_2 \frac{u_2v}{c^2} q_2$ neglecting terms $n_1 \frac{v^2}{2c^2} q_1$ and $n_2 \frac{v^2}{2c^2} q_2$ because they nearly cancel. This increase in charge density equals $\frac{v}{c^2} J$ in agreement with the second law of electromagnetic fields introduced in *The external electromagnetic field equations* section of this Appendix.

APPENDIX D. The gravitational field in non-relativistic quantum mechanics.

Although the gravitational field does not feature in most accounts of non-relativistic quantum mechanics it can of course have observable effects. We know, for example that any free quantum mechanical particle or particle system (such as a single atom) near the surface of the earth falls (like any free classical particle) with an acceleration of 1-g. And the earth's gravity has been found to affect the motion of neutrons in slow neutron interferometers. Therefore we need to introduce macroscopic sources of gravitational fields just as we introduced macroscopic sources of electromagnetic fields in Appendix C. But this time only sources of gravitational *scalar* potential are needed.* The only gravitational *vector* potential that may be present in our theory is a (source-less) constant background vector potential \mathbf{A}_0 accompanying a (source-less) constant background scalar potential V_0 as described in section 1 of Chapter III.

Quantum mechanical mass and system potentials

A quantum mechanical particle always carries a (non-zero and positive) mass. And this we suppose acts as a source of gravitational scalar potential much in the same way as a charged particle acts as a source of electromagnetic scalar potential.†

Particle masses are responsible for (gravitational) quantum mechanical inter-particle potentials and for quantum mechanical particle scalar potentials in any external gravitational field produced by macroscopic sources. Let the masses carried by the N particles of a system be m_i $i = 1, \dots, N$ and let the particle coordinates in a fixed coordinate system O be \mathbf{r}_i $i = 1, \dots, N$. With respect to O , if the gravitational potential of the external gravitational field is $\phi(\mathbf{r}, t)$ (which may include a contribution from the constant background potential V_0), then in the formula for the system potential in (2.1) of Chapter V, we will have (in the absence of potentials other than gravitational)

$$V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) = -G \frac{m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (\text{D.1})$$

where G is a constant ($G = 6.672 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$), and

$$V_i(\mathbf{r}_i, t) = m_i \phi(\mathbf{r}_i, t). \quad (\text{D.2})$$

* We do not suppose that there are gravitational *vector* potentials due to sources.

† Therefore we are able to model (fully and quantum mechanically) macroscopic sources of gravitational fields.

Also, as we have said before (see section 1 of Chapter III) if a constant background external gravitational vector potential field A_0 is present in O each particle experiences a constant quantum mechanical vector potential A_i given by

$$A_i = m_i A_0. \quad (D.3)$$

The external gravitational field equations

In non-relativistic quantum mechanics external gravitational fields are the product of macroscopic matter (forming macroscopic sources). The essential properties of that matter and the gravitational fields it produces are (like the kinematic properties of coordinate systems) not subject to the uncertainty principle.

For use in connection with non-relativistic quantum mechanics we state the following three laws governing the sources and their fields relative to any rest frame O in which position is denoted by \mathbf{r} and the time by t .

Law 1. There is distributed and effectively continuous macroscopic (and generally moving) mass of density $\rho(\mathbf{r}, t)$ and we suppose (in our modelling) that this density is under our control. The source density is assumed to satisfy a conservation equation, according to which at any time t

$$\int \rho d\tau = M \quad (D.4)$$

where M is a constant (independent of t), the (volume) integral being over all space.

Law 2. If the macroscopic mass is supposed to move with an extra uniform velocity \mathbf{v} , and is coincident with its previous form at time $t=0$, then $\rho(\mathbf{r}, t)$ changes to $\rho(\mathbf{r} - \mathbf{v}t, t)$.

Law 3. The macroscopic mass source produces a scalar gravitational potential field $\phi(\mathbf{r}, t)$ in O according to the rule*

$$\phi = -G \int \frac{\rho}{r} d\tau, \quad (D.5)$$

which gives the potential ϕ at any point P in O and at any moment in time. In (D.5) ρ is the mass density at the time in question and r is the distance from P to the general spatial volume element $d\tau$ in the integral.

* This is the same as the well known formula for the gravitational potential field of classical mechanics.

It follows from the relations ((D.2) and (D.3)) between the gravitational potentials and the quantum mechanical potentials, that when a single quantum mechanical particle of mass m moves *in the classical limit* (see section 1 of Chapter III) in an external gravitational field specified by potential field ϕ , it does so as if it obeyed Newton's second law of motion and experienced a force \mathbf{F} given by

$$\mathbf{F} = -m\nabla\phi \quad (\text{D.6})$$

where ϕ is the potential in the vicinity of the point occupied by the particle at the time in question. The result (D.6) is of course in agreement with the classical law.

Galilean invariance of the external field equations

We can prove that the external gravitational field equations are Galilean invariant.

The transformation equations under a velocity boost of coordinates are

$$\mathbf{F} = \mathbf{F}' \quad (\text{D.7})$$

$$m_i = m'_i \quad (\text{D.8})$$

$$\rho = \rho' \quad (\text{D.9})$$

$$\phi = \phi' \quad (\text{D.10})$$

((D.7) referring to (D.6)). And the same laws (D.4)-(D.6) apply under this transformation which is from coordinates O' to coordinates O , where O' moves with constant velocity \mathbf{v} , the origin of O' being at $\mathbf{v}t$ at time t . The un-primed variables on the LHS of (D.7)-(D.10) refer to position \mathbf{r} in O at time t and the primed variables on the RHS to position \mathbf{r}' in O' at time t with $\mathbf{r}' = \mathbf{r} - \mathbf{v}t$.

Note that (D.8) and (D.9) follow from the assumed absolute character of mass. (D.10) results from (D.5) applied to O' (to give $\phi' = -G\int(\rho'/r)d\tau$) and (D.9). And (D.7) results from (D.6), (D.8) and (D.10).

The external gravitational force field equations

We can define the gravitational force field \mathbf{g} as

$$\mathbf{g} = -\nabla\phi. \quad (\text{D.11})$$

From (D.5) it follows that

$$\nabla^2\phi = 4\pi G\rho, \quad (\text{D.12})$$

and therefore that

$$\nabla.\mathbf{g} = -4\pi G\rho. \quad (\text{D.13})$$

And (D.11)-(D.13) are the same as the gravitational field equations in classical mechanics.

The effective force (D.6) on a quantum mechanical particle of mass m in the classical limit becomes

$$\mathbf{F} = m\mathbf{g} \quad (\text{D.14})$$

which is the classical law.

The transformation equation for the gravitational force field under a velocity boost of coordinates is, by (D.11) and (D.10) simply

$$\mathbf{g} = \mathbf{g}' \quad (\text{D.15})$$

The internal gravitational field equations

In any quantum mechanical system (e.g. a hydrogen atom) there is an internal gravitational field. The sources of this field are the masses of the particles themselves. If the i^{th} particle has charge m_i it causes an internal gravitational potential at position \mathbf{r} in O given, at any time t , by

$$\phi_i = -G \frac{m_i}{|\mathbf{r} - \mathbf{r}_i|}$$

where \mathbf{r}_i is the position of the i^{th} particle at time t . It is this potential that gives rise to the inter-particle potential V_{ij} in (D.1). Since the value of \mathbf{r}_i is generally unknown and subject to the uncertainty principle, so is the value of ϕ_i at any given point \mathbf{r} .

In non-relativistic quantum mechanics the internal gravitational potential can be thought of as quasi-static (like the electric potential due to the charges of particles). The particles of a quantum mechanical system are moving at speeds small compared to the speed of light and, as we have said, they are assumed not to generate gravitational vector potential fields (even weakly).

When considering the total gravitational field we should of course include the internal gravitational potential field along with any external gravitational potential that may be present. Accordingly the total gravitational scalar potential at any point P and any time t is given by

$$\phi = -G \int \frac{\rho}{r} d\tau - G \sum_i \frac{m_i}{|\mathbf{r} - \mathbf{r}_i|} + V_0, \quad (\text{D.16})$$

in place of (D.5). Here \mathbf{r} is the position coordinate of P, r is the distance from P to the general volume element $d\tau$ and ρ is the mass density of the macroscopic source.

We note that since the \mathbf{r}_i may be non-differentiable functions of the time, $\partial\phi/\partial t$ is now generally non-existent. But this is of no consequence. The *spatial* derivatives, i.e. $\nabla\phi$, still exist (except at the positions of the particles themselves). So does the gravitational force field (as defined in (D.11)). The Galilean transformation equations (D.7)-(D.10) remain demonstrable. And so do the gravitational force field equations (D.11)-(D.13) with ρ now replaced by

$$\rho + \sum_i m_i \delta(\mathbf{r} - \mathbf{r}_i).$$

Orders of magnitude

Using a large enough mass source we can, at least in theory, produce a strong gravitational field to interact with a quantum mechanical system, and by varying the mass density or by moving the mass sources, we can produce time varying fields. We can, for example, model the fall of atoms or molecules in the combined gravitational fields of the earth and moon.

As is well known, the magnitude of the gravitational inter-particle potentials (compared with the electrostatic inter-particle potentials of charged particles) is far too small to be worth modelling. Take for example the case of a system consisting of two protons. The gravitational inter-particle potential is given by (D.1) and is of the order Gm^2/r while the electrostatic inter-particle potential is given by (C.1) of Appendix C, or in MKS units by

$$V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) = \frac{q_i q_j}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|}.$$

The order of magnitude of the latter is $q^2/(4\pi\epsilon_0 r)$. The ratio of the order of magnitudes is therefore $4\pi\epsilon_0 Gm^2/q^2$ where $G = 6.67 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$, $m = 1.67 \times 10^{-27} \text{ kg}$, $q = 1.6 \times 10^{-19} \text{ C}$ and $\epsilon_0 = 8.85 \times 10^{-12} \text{ F m}^{-1}$, giving $4\pi\epsilon_0 Gm^2/q^2 \approx 8.08 \times 10^{-37}$ which is far too small for inter-particle gravitational potentials to be of any significance in atomic and molecular theory. However, we should retain the idea that quantum mechanical particles produce gravitational potential fields, because this enables us to model macroscopic sources of gravitational potential which on account of the huge number of particles making up a large body like the earth *are* significant.

The second law of potential action

Relative to inertial frame O considered to be at rest, let $\phi(\mathbf{r}, t)$ be the gravitational potential field generated by (macroscopic) sources. These give rise, by (D.2), to quantum mechanical external potentials

$$V_i(\mathbf{r}_i) = m_i \phi(\mathbf{r}_i, t) \tag{D.17}$$

on the i^{th} particle of a quantum mechanical system. We have postulated in law 2 above that if the source mass distribution is given a velocity boost \mathbf{v} but is the same at time $t=0$ then the source density changes from $\rho(\mathbf{r}, t)$ to $\rho(\mathbf{r} - \mathbf{v}t, t)$. By (D.5) the potential field $\phi(\mathbf{r}, t)$ thus changes to $\phi(\mathbf{r} - \mathbf{v}t, t)$. Accordingly the quantum mechanical potentials (D.17) change from $V_i(\mathbf{r}_i)$ to $V_i(\mathbf{r}_i - \mathbf{v}t)$. And since there is no vector potential in this case, this is in agreement with the second law of potential action (section 3.2 of Chapter III).

So when the external potentials are gravitational in origin the second law of potential action (section 3.2 of Chapter III) is a consequence of the gravitational field equations.

APPENDIX E. Results relating to section 8.2 of Chapter XIV

In this Appendix all equation numbers refer to Chapter XIV.

Proof of the uniqueness of μ .

The equation for μ is, by (8.2.9)

$$\frac{\sum_{nl} e^{-\mu E_n} E_n}{\sum_{nl} e^{-\mu E_n}} = \bar{E}$$

in which \bar{E} and the E_n are supposed known. We show the LHS is a monotonic decreasing function of μ and therefore can equal the RHS only for one value of μ .

To show that the LHS is monotonic decreasing we differentiate it with respect to μ getting

$$-\frac{\sum_{nl} e^{-\mu E_n} E_n^2}{\sum_{nl} e^{-\mu E_n}} + \left(\frac{\sum_{nl} e^{-\mu E_n} E_n}{\sum_{nl} e^{-\mu E_n}} \right)^2$$

which equals

$$-\frac{\sum_{nl} e^{-\mu E_n} (\bar{E} - E_n)^2}{\sum_{nl} e^{-\mu E_n}}$$

which is negative for all μ . QED.

Proof that λ and μ derived from (8.2.9) make S in (8.2.5) a maximum

We use the method given by Jaynes (pp 45-47 of [28]). Accordingly we start with the fact that

$$\ln x \geq 1 - \frac{1}{x} \quad \text{for all } x > 0^*$$

* Note that the curves $\ln x$ and $1 - \frac{1}{x}$ touch one another at $x = 1$ without crossing each other.

the equality holding only when $x=1$. This means that for any distribution w'_{nl} satisfying the constraints (8.2.6) but differing from the w_{nl} given by (8.2.8)

$$\sum_{nl} w'_{nl} \ln \frac{w'_{nl}}{w_{nl}} \geq \sum_{nl} w'_{nl} \left(1 - \frac{w_{nl}}{w'_{nl}}\right)$$

the equality holding only when $w'_{nl} = w_{nl}$ for all nl . Substituting for w_{nl} as given by (8.2.8), i.e. putting $w_{nl} = e^{-\lambda - \mu E_n}$ on the LHS we get

$$\sum_{nl} w'_{nl} \ln w'_{nl} - \sum_{nl} w'_{nl} (-\lambda - \mu E_n) \geq \sum_{nl} (w'_{nl} - w_{nl})$$

or

$$\sum_{nl} w'_{nl} \ln w'_{nl} + \lambda + \mu \bar{E} \geq 0.$$

Therefore

$$-\sum_{nl} w'_{nl} \ln w'_{nl} \leq \lambda + \mu \bar{E}.$$

Here the LHS is the value of the information entropy going with the w'_{nl} and the RHS is the value of the information entropy for w_{nl} given by (8.2.8) because

$$-\sum_{nl} w_{nl} \ln w_{nl} = -\sum_{nl} w_{nl} (-\lambda - \mu E_n) = \lambda + \mu \bar{E}.$$

Therefore λ and μ derived from (8.2.9) make w_{nl} (as given by (8.2.8)) *maximise* S in (8.2.5). QED.

APPENDIX F. Expected frequencies and actual frequencies

The relationship between *expected* frequencies (derived using classical probability theory) and *actual* frequencies is much discussed in [2] (see for example Chapter 9 of [2]). But it will be useful to reconsider this question here. To this end we consider a specially constructed example in classical probability and we rework this example using complex-valued probability theory instead. Finally we consider what we should do if actual frequencies differ from expected frequencies.

A specially constructed example in classical probability

Suppose we have written a computer program that outputs the following determinate sequence of zeros and ones

01 011 00 01 10 11 011 011 000 001 010 100 011 101 110 111 011 011 011 011 011 011
0000 0001

constructed as follows. The program outputs all possible ways of writing zeros and ones first signally, then in an ordered pair, then in an ordered set of three, then in an ordered set of four etc (these are the underlined digits in the sequence). But between these the program enters 011 first once, then 2! times, then 3! times etc.

We define a process P_N of order N ($N = 1, 2, 3, \dots$) as one resulting in a string of N consecutive digits selected at random from this sequence. For example, with $N = 4$, the process when 'run' could give 0101 (the first four consecutive digits) or 0011 (the 7th to 10th consecutive digits) or any four consecutive digits in the sequence. By the construction of the sequence we see that

- (i) A process P_N may result in *any* ordered set of N numbers (each number being a zero or a one).
- (ii) For $N \rightarrow \infty$ the relative frequency (or relative number) of zeros is $1/3$ and that of ones $2/3$.

For example (i) is satisfied when $N = 3$ because a process of order 3 could start at any point in the third underlined part of the sequence and so result in any given ordered triplet of zeros and ones. By the construction of the sequence it is clear that (i) is satisfied just as well for any value of N . Also (ii) is evidently satisfied because for large N , wherever the process starts, many more cases of the not-underlined digits will occur than of the underlined digits, and the more so the larger N .

Now suppose we give to somebody else (person B) the knowledge Y that a certain physical process 'of order N ' will be run resulting in one of 2^N possible outcomes and that these possible outcomes are numbered using binary numbers $r_1 \dots r_N$ each r being either 0 or 1. Thus the binary numbers representing the possible outcomes range from

$r_1 \dots r_N = 00 \dots 0$ (all zeros) to $r_1 \dots r_N = 11 \dots 1$ (all ones).

Person B does not know that the digits in the binary number will be a series of N consecutive digits *drawn at random from our series*. Nonetheless we can ask person B to calculate their probability for the digit r_1 being 1. Similarly we can ask person B for their probability for r_1 being 1 *and* r_2 being 0. In fact we can ask for the probability of any proposition concerning r values in the binary number representing the outcome of the process. Person B calculates their probabilities on the basis only of the information Y we have provided.

Applying classical rational-Bayesian probability theory person B assigns, by the principle of indifference, equal probabilities to each of the 2^N possible outcomes of the process. Accordingly person B gets, for any ordered set $r_1 \dots r_N$ of r values, the probability

$$P(r_1 \dots r_N | Y) = \frac{1}{2^N} \quad (\text{F.1})$$

Person B then calculates, using the sum rule, that the probability for a particular value of (say) r_1 is

$$P(r_1 | Y) = \sum_{r_2 \dots r_N} P(r_1 \dots r_N | Y) = \sum_{r_2 \dots r_N} \frac{1}{2^N} = \frac{1}{2^N} \times 2^{N-1} = \frac{1}{2}. \quad (\text{F.2})$$

Similarly person B gets, for the probability of any particular values of r_1 and r_2 the result

$$P(r_1 r_2 | Y) = \sum_{r_3 \dots r_N} P(r_1 \dots r_N | Y) = \frac{1}{2^N} \times 2^{N-2} = \frac{1}{2^2} \quad (\text{F.3})$$

and they find

$$P(r_1 r_2 r_3 | Y) = \sum_{r_4 \dots r_N} P(r_1 \dots r_N | Y) = \frac{1}{2^N} \times 2^{N-3} = \frac{1}{2^3} \quad (\text{F.4})$$

...etc. And using the fact that the probability of each outcome is $1/2^N$ and employing the sum rule, person B can also deduce in the familiar manner that the probability for exactly n zeros in the binary number labelling the outcome of a process of order N is

$$P(n \text{ zeros} | Y) = {}_N C_n \left(\frac{1}{2}\right)^n \left(\frac{1}{2}\right)^{N-n} \quad (\text{F.5})$$

and hence, as $N \rightarrow \infty$, that the expected relative frequency (or relative number) of zero digits in the binary number is $1/2$. That is one-half of the digits are expected to be zero. More precisely person B can deduce that given any fixed positive number δ however

small the probability that the frequency of zero digits lies inside the range $\frac{1}{2} - \delta$ to $\frac{1}{2} + \delta$ tends to one as $N \rightarrow \infty$.

The same example using complex-valued probability

The above result can just as well be derived by applying complex-valued probability. In place of (F.1) person B then writes (from the complex-valued form of the principle of indifference) that

$$\Phi(r_1 \dots r_N | Y) = \frac{1}{\sqrt{2^N}} e^{i\alpha}$$

where the phase α is independent of the $r_1 \dots r_N$ values because B is absolutely indifferent with regard to which of the outcomes might occur. Person B's degree of belief for $r_1 \dots r_N$ is thus

$$|\Phi(r_1 \dots r_N | Y)|^2 = \frac{1}{2^N}$$

the same as in the classical probability case.

Using the complex-valued form of the sum rule, person B then derives all the same formulae (F.2)-(F.5) with $P(\cdot)$ replaced by $|\Phi(\cdot)|^2$. And person B deduces that for $N \rightarrow \infty$ their expected relative frequency (or relative number) of zero digits in the binary number is $\frac{1}{2}$, or their degree of belief for a relative frequency of zero digits inside the range $\frac{1}{2} - \delta$ to $\frac{1}{2} + \delta$ tends to one as $N \rightarrow \infty$. So again, one-half of the digits are expected to be zero. The phase of belief associated with this degree of belief is indeterminate because of the use of the sum rule in the calculations and the fact that person B cannot claim their knowledge is pure and that α has a determinate value.

An advantage of complex-valued probability

The above example shows clearly that an *expected* frequency (correctly calculated from the laws of classical or complex-valued probability) may be quite different from the *actual* frequency. Expected frequencies depend on the extent of our knowledge while actual frequencies do not.

In classical probability theory, when the probability of a proposition is equal to 1 this is usually interpreted as meaning the proposition in question is certainly true. But in that case person B, in the above example, could *prove* that the actual frequency of zero values for $N \rightarrow \infty$ was $1/2$ and this would be in contradiction to the actual value of $1/3$. This is a major problem because clearly somebody with valid knowledge should not be able to prove something false!

When applying our *complex-valued* probability theory to the same example the situation is clearer. For although our degree of belief for the expected outcome frequency

is equal to 1 in the limit $N \rightarrow \infty$, our associated phase of belief is necessarily *indeterminate*. So we are unable to claim the expected frequency must *certainly* be the actual frequency in the limit $N \rightarrow \infty$. We can claim only that we *logically expect* a particular frequency to be present (as $N \rightarrow \infty$) with the (usual) caveat that this expectation is based on limited knowledge and could be wrong. The thing is that in our complex-valued probability theory (which is supposed to be universally applicable) we have a *mathematical* way of distinguishing certainty from expectation, while no such way is present in classical probability theory.

What to do if actual frequencies differ from expected frequencies

If person B is told the numbers of zeros and ones in each binary number obtained when many particular processes of larger and larger orders are run, they will soon notice that the relative frequency of zero digits in the binary number is close to $1/3$ for large N and generally approaches $1/3$ more and more closely as N increases. How then should person B react? Person B should first check their calculations and when these are found to be perfectly correct, person B should consider that they have more to learn about the nature of the process in question. They may choose to postulate certain additional physical properties of the process which taken together with the knowledge they already had would lead to the calculation (for $N \rightarrow \infty$) of an expected relative frequency of zero digits of $1/3$ rather than $1/2$.

Given *pure* knowledge of a *quantum mechanical* process, we have seen in section 9 of Chapter II how expected frequencies of outcomes (i.e. of certain possessed properties of the system in question) in repeated trials of that process can be rigorously calculated on the basis of complex-valued probability theory. In that calculation use is made of the law of absolute logical independence under pure knowledge. Under pure knowledge we cannot generally claim that our expected frequencies are indicative of actual frequencies of the outcomes in a large number of trials. We do however expect the observed results in many trials to conform approximately to the expected frequencies and *generally* more and more closely so as the number of trials increases. If this is found not to be the case we may consider we have reason to doubt the validity of our logical reasoning or to doubt the validity of the physical assumptions we have made before applying probability theory to the process in question. Only in this sense are probabilistic predictions of quantum theory confirmable (or not) by observations. Happily, provided we adopt the correct laws of probability (or of logic in general) and make the correct physical assumptions, agreement is achieved well enough and we have no reason to worry.

APPENDIX G. Evolution of a wave function initially zero in one half of space and of unit value in the other

We consider the evolution in free space of a single particle wave function $\psi(\mathbf{r}, t)$ (referred to a fixed coordinate system) which initially (at time $t=0$) is zero for $x > 0$ and equal to 1 for $x < 0$. Clearly $\psi(\mathbf{r}, t)$ will be a function $\psi(x, t)$ only of the particle's x coordinate and of the time t . And $\psi(x, t)$ must satisfy the Schrödinger equation

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad (\text{G.1})$$

for $t > 0$, and at time $t=0$ we have

$$\psi = \psi_0 = \begin{cases} 0 & x > 0 \\ 1 & x < 0 \end{cases} \quad (\text{G.2})$$

Applying the Laplace transform method (see for example [23]), we put

$$\bar{\psi} = \int_0^{\infty} \psi e^{-pt} dt \quad (\text{G.3})$$

with inverse formula

$$\psi = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \bar{\psi} e^{pt} dp \quad (\text{G.4})$$

where the (real) constant γ may take any value greater than the real parts of the singularities of $\bar{\psi}$, and the integral is along the contour parallel to the imaginary axis passing through $(\gamma, 0)$. Multiplying (G.1) through by e^{-pt} and integrating over t from 0 to ∞ (using integration by parts in the case of the term $\frac{\partial \psi}{\partial t}$) gives

$$\begin{aligned} \frac{\partial^2 \bar{\psi}}{\partial x^2} &= -i\alpha^2 p \bar{\psi} & x > 0 \\ \frac{\partial^2 \bar{\psi}}{\partial x^2} + i\alpha^2 p \bar{\psi} &= i\alpha^2 & x < 0 \end{aligned} \quad (\text{G.5})$$

where

$$\alpha = \sqrt{\frac{2m}{\hbar}}. \quad (\text{G.6})$$

The solutions of (G.5) finite for $x \rightarrow \infty$ and $x \rightarrow -\infty$ respectively are

$$\begin{aligned} \bar{\psi} &= Ae^{-\alpha\sqrt{-ip}x} & x > 0 \\ \bar{\psi} &= Be^{\alpha\sqrt{-ip}x} + \frac{1}{p} & x < 0 \end{aligned} \quad (\text{G.7})$$

the cut for the square root function being along the negative real axis of the complex plane so that for example

$$\sqrt{-i} = \frac{1}{\sqrt{2}}(1-i)$$

and \sqrt{p} will have a non-negative real part whatever the value of γ . Imposing the boundary condition that $\bar{\psi}$ (and its first derivative in x) be continuous at $x=0$ we find $A = -B = \frac{1}{2p}$ so by (G.7)

$$\begin{aligned} \bar{\psi} &= \frac{1}{2p}e^{-\alpha\sqrt{-ip}x} & x > 0 \\ \bar{\psi} &= -\frac{1}{2p}e^{\alpha\sqrt{-ip}x} + \frac{1}{p} & x < 0 \end{aligned} \quad (\text{G.8})$$

From a table of Laplace transforms (p.229 and p.245 of [24]) we thus find

$$\begin{aligned} \psi &= \frac{1}{2}\text{erfc}\left(\frac{1}{2}\alpha\sqrt{-i}xt^{\frac{1}{2}}\right) & x > 0 \\ \psi &= \frac{1}{2}\text{erfc}\left(-\frac{1}{2}\alpha\sqrt{-i}xt^{\frac{1}{2}}\right) + 1 & x < 0 \end{aligned} \quad (\text{G.9})$$

or using the relations

$$\begin{aligned} \text{erfc}(z) &= 1 - \text{erf}(z) \\ \text{erf}\left(\frac{\sqrt{\pi}}{2}(1-i)z\right) &= \frac{2}{1+i}(C(z) + iS(z)) \end{aligned}$$

(see for example p.297 and p.301 of [21]) where $C(z)$ and $S(z)$ are Fresnel integrals defined and graphed in [21], we arrive at the solution of the problem in the more manageable form

$$\psi = \frac{1}{2}\left(1 - \frac{2}{1+i}\left(C\left(\frac{\alpha x}{\sqrt{2\pi t}}\right) + iS\left(\frac{\alpha x}{\sqrt{2\pi t}}\right)\right)\right) \quad -\infty < x < \infty \quad (\text{G.10})$$

A plot of the real and imaginary parts of the RHS of (G.10) together with the step form of ψ at time $t=0$ is given in Figure G.1.

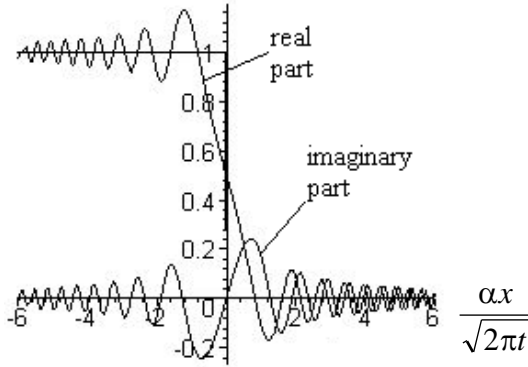


Figure G.1

The form of ψ from time $t=0$ changes markedly only for say $|\alpha x/\sqrt{2\pi t}| < 10$ i.e. for $-10\sqrt{2\pi t}/\alpha < x < 10\sqrt{2\pi t}/\alpha$. For short times this is but a small range and smaller and smaller the shorter the time.

If we define the probability (or rather degree of belief) current density i by

$$i = \frac{i\hbar}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi)$$

as on p.57 of [12], we have in relation to ψ in (G.10) that

$$i_x = \frac{i\hbar}{2m}(\psi \frac{\partial\psi^*}{\partial x} - \psi^* \frac{\partial\psi}{\partial x}).$$

Evaluating this at $x=0$ we find

$$i_x|_{x=0} = \frac{1}{4} \sqrt{\frac{\hbar}{m\pi t}}.$$

The flux of degree of belief (from $x < 0$ to $x > 0$) across unit area of the yz plane from time $t=0$ to time $t=\delta$ is therefore

$$\int_0^\delta i_x|_{x=0} dt = \frac{1}{2} \sqrt{\frac{\hbar}{m\pi}} \delta.$$

So this flux is small for small δ and grows only as the square root of δ .

APPENDIX H. Classical probability applied to Brownian motion

Consider the classical motion of a dilute suspension of very tiny (classically identical) particles in an unbounded stationary fluid (Brownian motion). Since the suspension is *dilute*, the motion of any particular particle proceeds in a manner physically independent of the motion of the others. Let $\rho(\mathbf{r}, t)$, which we write as $\rho(\mathbf{r}t)$ for short, be the probability density for the particle position \mathbf{r} at time t .

In a way that closely resembles our derivation of the free particle Schrödinger equation in section 2 of Chapter IV using complex-valued probability, we can derive a differential equation (the diffusion equation) for $\rho(\mathbf{r}t)$ using classical probability on the basis of the following assumptions.

- (i) Space is homogeneous and isotropic and time is homogeneous.
- (ii) The particle does not move infinitely fast.
- (iii) Relative to fixed Cartesian coordinates, the x, y and z components of the motion of the particle are logically independent. So for example, propositions about the x component of motion of the particle are logically independent of propositions about the y and z components of the motion.
- (iv) There is just one quantity physically characterising the motion of the particle. This is the real and positive ‘diffusion coefficient’ which has units L^2T^{-1} but whose actual value (for any given fluid) we take to be unknown.

We first seek the probability distribution $P(d^3\mathbf{r}_2t_2 | d^3\mathbf{r}_1t_1)$ for the particle to be in volume element $d^3\mathbf{r}_2$ at time t_2 given it was in volume element $d^3\mathbf{r}_1$ at time t_1 ($< t_2$). We can write this as

$$P(d^3\mathbf{r}_2t_2 | d^3\mathbf{r}_1t_1) = f(\mathbf{r}_2t_2; \mathbf{r}_1t_1) d^3\mathbf{r}_2 \quad (\text{H.1})$$

where

$$\int f(\mathbf{r}_2t_2; \mathbf{r}_1t_1) d^3\mathbf{r}_2 = 1. \quad (\text{H.2})$$

From assumption (i) above we deduce the form

$$f(\mathbf{r}_2t_2; \mathbf{r}_1t_1) = f(\mathbf{r}_2 - \mathbf{r}_1, t_2 - t_1) = f(\mathbf{R}, \tau)$$

where $\mathbf{R} = \mathbf{r}_2 - \mathbf{r}_1$ and $\tau = t_2 - t_1$. This is shown in exactly the same way that (1.6) in Chapter IV was shown.

Rotations form a transformation group so, following the steps leading to (1.8) of

Chapter IV, we must similarly have

$$f(\mathbf{R}, \tau) = f(|\mathbf{R}|, \tau).$$

The form of (H.1) means that $f(|\mathbf{R}|, \tau)$ must have dimensions L^{-3} . But the only quantities at our disposal are $|\mathbf{R}|, \tau$ and the diffusion coefficient which we denote by D . So dimensional analysis gives us $f(|\mathbf{R}|, \tau) = (D\tau)^{-3/2} h(R^2/D\tau)$, or since $f(|\mathbf{R}|, \tau)$ is positive we can write

$$f(|\mathbf{R}|, \tau) = (D\tau)^{-3/2} \exp(g(R^2/D\tau)). \quad (\text{H.3})$$

where g is some real-valued function.

The linearity of g can be demonstrated using assumption (iii). The steps in the derivation of (H.3) are repeated for the logically independent x, y and z components of the motion. The distributions

$$f_1(|x|, \tau) = (D\tau)^{-1/2} \exp(g_1(\frac{x^2}{D\tau}))$$

$$f_2(|y|, \tau) = (D\tau)^{-1/2} \exp(g_2(\frac{y^2}{D\tau}))$$

$$f_3(|z|, \tau) = (D\tau)^{-1/2} \exp(g_3(\frac{z^2}{D\tau}))$$

result in which, by *similarity*, the functions g_i (for $i=1,2,3$) are all one and the same function. The product of these distributions for the component motions must equal $f(|\mathbf{R}|, \tau)$ in (H.3). As a result

$$g(\frac{R^2}{D\tau}) = g(\frac{x^2 + y^2 + z^2}{D\tau}) = g_1(\frac{x^2}{D\tau}) + g_1(\frac{y^2}{D\tau}) + g_1(\frac{z^2}{D\tau})$$

and this implies

$$g(\frac{R^2}{D\tau}) = \frac{A}{D\tau} (x^2 + y^2 + z^2) + B$$

where A and B are real constants. So we find

$$f(\mathbf{r}_2 t_2; \mathbf{r}_1 t_1) = (D\tau)^{-3/2} \exp(\frac{A}{D\tau} (x^2 + y^2 + z^2) + B)$$

where, by assumption (ii) A must be negative.

Now $f(\mathbf{r}_2 t_2; \mathbf{r}_1 t_1)$ has to satisfy (H.2), and using the result

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}},$$

for $a > 0$ we find $e^B (\pi/(-A))^{3/2} = 1$ and therefore

$$f(\mathbf{r}_2 t_2; \mathbf{r}_1 t_1) = \left(\frac{\pi D \tau}{\alpha}\right)^{-3/2} \exp\left(-\frac{\alpha}{D \tau} (x^2 + y^2 + z^2)\right) \quad (\text{H.4})$$

where $\alpha (= -A)$ is a positive constant.

Since we do not know the value of D the constant α can be absorbed into D or set equal to any positive real number. We choose to put $\alpha = 1/4$ and finally obtain

$$f(\mathbf{r}_2 t_2; \mathbf{r}_1 t_1) = (4\pi D \tau)^{-3/2} \exp\left(-\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{4D \tau}\right). \quad (\text{H.5})$$

This closely resembles the result (1.20) of Chapter IV.

Now given the probability density $\rho(\mathbf{r}_1 t_1)$ for the particle position at time t_1 , the probability density $\rho(\mathbf{r} t)$ at time t later on will, by the sum and product rules of classical probability, clearly be

$$\rho(\mathbf{r} t) = \int \rho(\mathbf{r}_1 t_1) f(\mathbf{r} t; \mathbf{r}_1 t_1) d^3 \mathbf{r}_1 \quad (\text{H.6})$$

and since the distribution $f(\mathbf{r} t; \mathbf{r}_1 t_1)$ given by (H.5) satisfies the differential equation

$$\frac{\partial f}{\partial t} - D \nabla^2 f = 0$$

so too does $\rho(\mathbf{r} t)$. That is, the general probability density $\rho(\mathbf{r} t)$ for particle position must always satisfy the differential equation

$$\frac{\partial \rho}{\partial t} - D \nabla^2 \rho = 0 \quad (\text{H.7})$$

This completes the derivation of the differential equation for $\rho(\mathbf{r} t)$ in which we may determine the value of D from experiments.

APPENDIX I. The geometric representation of propositions, phases of implication and phases characteristic of knowledge

In order to visualise propositions and picture how (in the new logic) one proposition might imply another *with a phase of implication*, we construct an (extended) Venn diagram with an intrinsic ‘metric’ and equate phases of implication to metrical properties in the diagram. We put into 1-1 correspondence abstract concepts in the new logic with geometrical concepts in the Venn diagram. And in this way we provide a degree of confidence in the feasibility and consistency of the general rules we claim (in the main text) for phases of implication and phases characteristic of knowledge.

Introduction

By way of introduction we first consider an ordinary Venn diagram in the plane (Figure I-1). Here propositions A, B, \dots etc. claiming dynamical properties of the physical world, are represented by regions within a region P . We can think of each point (or tiny region) of P as representing a ‘possible world’, i.e. a possible (hypothetical) history of all dynamical properties of the physical world expressed to quantum mechanical accuracy. Any proposition, such as A , claims that one of the possible worlds within region A is the actual world. The proposition represented by P is thus the proposition which makes no specific claim regarding which (out of all the worlds known to be possible) is the actual world.

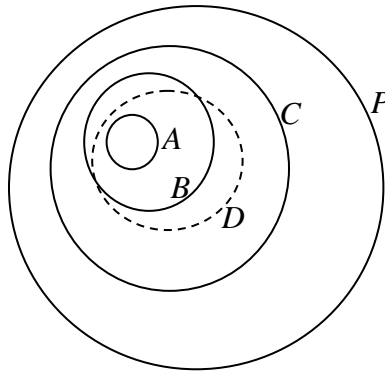


Figure I-1

If one proposition implies another, the region representing the first lies entirely within the region representing the second (so for example $A \Rightarrow B$ in Figure I-1). It is geometrically evident that if $A \Rightarrow B$ and $B \Rightarrow C$ then $A \Rightarrow C$. Further, if we identify the area between A and B (measured modulo 2π) with the phase of implication with which A implies B then it is clear that if $A \Rightarrow^\alpha B$ and $B \Rightarrow^\beta C$ then $A \Rightarrow^{\alpha+\beta} C$ as we have

claimed in (2.2.1.2) of Chapter I.

We note that if $A \Rightarrow^\delta D$ and $D \Rightarrow^\varepsilon C$ (where D differs from B) then we deduce that $A \Rightarrow^{\delta+\varepsilon} C$. And this is consistent with $A \Rightarrow^{\alpha+\beta} C$ because of the geometrical equality $\delta+\varepsilon=\alpha+\beta$. We note also that instead of employing the actual area between propositions to represent the phase of implication we can introduce a metric or notional density (generally non-uniform) over the plane and employ the notional *weighted* area (the area weighted by the density*) between the propositions (again measured modulo 2π). Clearly that would do just as well, and there are any number of different ways of measuring phases of implication in this way according to the manner in which the density varies from point to point over the plane, and it may vary in a continuous or discontinuous way.

Extension of the Venn diagram

But in this ‘model’, if two propositions are equivalent (i.e. represented by the same region in the Venn diagram) they must imply one another with zero phase of implication since the area (weighted or not) between the representative regions is zero. We therefore need to modify the model somehow to accommodate equivalence with non-zero phases of implication. This we do by extending the Venn diagram into the

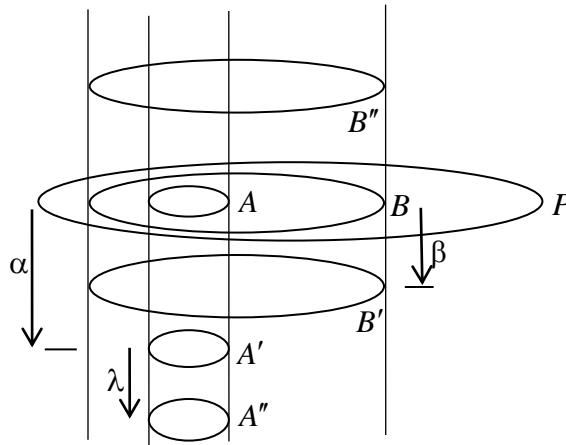


Figure I-2

third dimension. We claim (see Figure I-2) that there may be further propositions occupying positions in planes parallel to the plane of the original Venn diagram which we now refer to as the ‘home plane’. So propositions are represented not only by regions A or B , ...etc in the home plane but also by regions A', B', \dots etc. or A'', B'', \dots etc. which lie directly below or directly above what we call their ‘projections’ A, B, \dots etc in the

* or if you like, the ‘mass’ of the area.

home plane.* To measure the phases of implication between equivalent propositions (represented always by regions which lie directly above or below each other) we employ the vertical displacement between those propositions. In Figure I-2 for example we say $A' \overset{-\lambda}{\Leftrightarrow} A''$ where λ is the vertical distance A' to A'' measured positive downwards (modulo 2π). Or, introducing a new fixed metric or density (generally a function of distance below the home plane), we can say $A' \overset{-\lambda}{\Leftrightarrow} A''$ where λ is the weighted length[†] of any vertical line joining the plane occupied by region A' to the plane occupied by region A'' , and measured positive downwards (modulo 2π).

Clearly any one proposition implies another if its projection on the home plane lies within the projection of the other. For example, in Figure I-2, $A' \Rightarrow B'$, and we may say it does so with a phase of implication equal to $-\alpha + \gamma + \beta$ where $-\alpha$ is the phase with which A' implies A , γ is the phase with which A implies B , and β is the phase with which B implies B' . Here γ is the (weighted) area between A and B in the home plane and $-\alpha$ and β the (weighted) vertical displacements from A' to A , and from B to B' .

There seems now, however, little point in maintaining the dependence of phases of implication on the areas between the projections of propositions in the home plane. We may obtain any phase of implication we might want simply by changing the vertical positions of the propositions in question. At any rate, from now on we set the weighting of areas in the home plane equal to zero. So, for example, in Figure I-2 we say $A' \Rightarrow B'$, with a phase of implication equal to $-\alpha + \beta$.

The occupation of positions by propositions

Any proposition about dynamical properties of the physical world is supposed to occupy a position (i.e. an area in a horizontal plane at a certain height) in the Venn diagram. But it is possible that not *all* positions in the Venn diagram are occupied by propositions about dynamical properties of the physical world. However, it will be useful (and harmless) for labelling purposes, to consider all positions to be occupied by propositions even if some of the propositions occupying positions cannot be expressed in ordinary language. We call the latter kind of proposition 'unreal'.

With regard to any proposition A in the home plane whether that proposition be real or unreal, there is always of course a real proposition A' lying somewhere directly above or below its projection A . This proposition A' expresses in ordinary language the claim that one or other of the possible worlds covered by A is the actual world. As well as A' the propositions $A'A'$, $A'A'A'$, $A'+A'A'$, ... etc. are real propositions logically equivalent to A' (not necessarily *fully* equivalent to A') but not all propositions A'' with projection A are propositions expressible in ordinary language.

* Note that in this Appendix we distinguish, for clarity, propositions definitely on or normally off the home plane by using primed capitals for the latter and un-primed capitals for the former. This convention is not however used in the main text of the monograph. So in the main text a proposition with or without (one or more) primes should not be given the significance it would have in this appendix.

† or if you like, the 'mass'

Characteristic values

For the purpose of modelling phases characteristic of knowledge later on, and for the purpose of expressing phases of implication algebraically, we suppose there is a ‘characteristic value’ $c(A')$ of any proposition A' according to its vertical position in the (extended) Venn diagram. If the area occupied by the proposition A' lies in the home plane (so A' coincides with its projection A on that plane) then $c(A') = c(A)$ and

$$c(A) = 0. \tag{I.1}$$

If A' lies distance α below its projection A we define $c(A')$ as follows:

$$c(A') = \alpha, \text{ where } \alpha \text{ is the displacement of } A' \text{ below } A. \tag{I.2}$$

In (I.1) and (I.2) and henceforth, we take for granted that the vertical displacements are weighted (in a fixed way) without mentioning this every time. And we always measure the (weighted) displacements modulo 2π . So propositional characteristic values can have any real value modulo 2π :

$$-\infty < c(A') < \infty \quad \text{modulo } 2\pi. \tag{I.3}$$

This means that a proposition A'' related to A' by $A' \stackrel{-\lambda}{\Leftrightarrow} A''$ where $\lambda = 2\pi n$ (where n is any integer) is the same as proposition A' , or at least fully equivalent to it.

If $A' \Rightarrow B'$ we take it to do so with phase of implication given by the rule:

$$\text{If } A' \Rightarrow B', \text{ then } A' \Rightarrow^\mu B' \text{ where } \mu = c(B') - c(A') \text{ modulo } 2\pi. \tag{I.4}$$

But of course the converse is not generally true, i.e. given $c(B') - c(A') = \lambda$, it does not follow that $A' \Rightarrow^\lambda B'$ or even that $A' \Rightarrow B'$. We note that (I.4) demonstrates the feasibility of the claims (2.2.1.1) and (2.2.1.2) of Chapter I.

Any proposition which makes no claim, or no significant claim regarding dynamical properties because its truth is already known from our general knowledge* we identify with the proposition P in our Venn diagram, and we take *its* characteristic value to be zero modulo 2π . Thus

$$c(P) = 0 \text{ modulo } 2\pi. \tag{I.5}$$

So if one proposition P' making no real claim implies another proposition P'' making no real claim it does so with zero phase of implication (since P' and P'' are both identified with P), or in our Venn diagram there are no propositions P' lying directly above or directly below the proposition P in the home plane.

* For example the proposition claiming a particular particle in the physical world has one or other of all possible positions in space at a particular time.

The disjunction of two or more propositions

When propositions are positioned in the home plane, their disjunction is defined in the normal way. So the disjunction $A+B$ of A and B is represented by the area of the home plane covered by the regions representing A and B taken together.

To define the disjunction $A' + B'$ of two propositions A' and B' not necessarily on the home plane we introduce a *positive* weight for every atomistic proposition a_1, a_2, \dots in the home plane* and define the weight of any proposition A (in the home plane) as the sum of the weights of the atomistic propositions making it up. We denote the weight of A by w_A , the weight of B by w_B and so on. (If A and B are mutually exclusive then of course $w_{A+B} = w_A + w_B$, but we do not here assume that A and B are necessarily mutually exclusive). For reasons that will become apparent soon we need (notionally) to assign the weights to the atomistic propositions in a *certain kind of way*. We do it so that mutually exclusive propositions in the home plane always have weights of different orders of magnitude. For example we may take the weights to be as follows.

$$\left. \begin{array}{l} w_{a_1} = 0.1, \\ w_{a_2} = 0.01, \\ w_{a_3} = 0.001, \\ \dots \text{etc.} \end{array} \right\} \text{ and } \left. \begin{array}{l} w_A = \sum_{a_i \in A} w_{a_i}, \\ w_B = \sum_{a_i \in B} w_{a_i}, \\ \dots \text{etc.} \end{array} \right\} \quad (\text{I.6) and (I.7)}$$

Using these weights we define the disjunction $A' + B'$ in the following way. First we project A' and B' onto the home plane and form the disjunction $A+B$ of their projections (see Figure I-3 where $A^{-\alpha} \Leftrightarrow^{\alpha} A'$ and $B^{-\beta} \Leftrightarrow^{\beta} B'$).

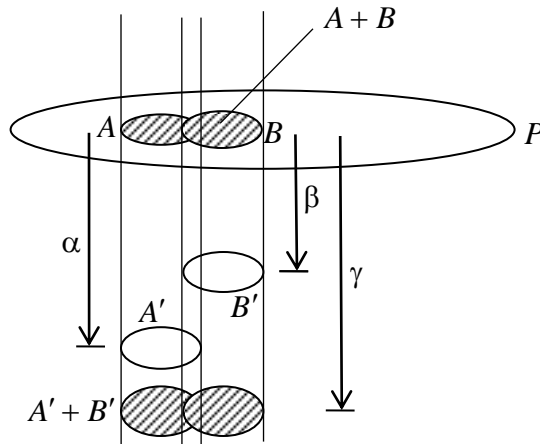


Figure I-3

* We picture these atomistic propositions as many small areas finite in number covering the home plane with the view that we can, if necessary, take the limit as their number tends to infinity.

We then move the area representing the disjunction $A+B$ down a distance γ given by

$$\gamma = \{\alpha, \beta; w_A, w_B\} \tag{I.8}$$

which is shorthand for saying that we take $\gamma = \alpha$ if $w_A > w_B$ and we take $\gamma = \beta$ if $w_B > w_A$. This displaced area represents the disjunction $A' + B'$. Note that the choice (I.6) for the weights of the atomistic propositions ensures that either $w_A > w_B$ or $w_A < w_B$ is true; indeed it ensures that every proposition in the home plane has a *unique* weight.

The only kind of disjunction that remains to be specified is the kind in which propositions A' and B' coincide or lie directly one below the other. Then $w_A = w_B$ and we need some other way to fix γ . We do it by expressing the drops α and β (of A' and B' below A and B) in the range $0 \leq \alpha < 2\pi$ and $0 \leq \beta < 2\pi$, putting γ equal to α or β according to which of α and β (so expressed) is the smallest (or, in another way, according to which of α and β (so expressed) is the largest). If α and β are equal we simply put γ equal to either one (for example to α).

The displacement, as given by (I.8) or by the rule just stated, is of course zero when A' and B' lie in the home plane (since α and β are then zero).

We now have a definite rule for formulating disjunctions of any two propositions. But we need to qualify it in one respect. For whenever the projections of the two propositions onto the home plane fill the region P , their disjunction can only be equal to P . It cannot equal P displaced up or down by some distance because by convention we rule out such locations for propositions. So, if the projections A and B of A' and B' fill P we take the disjunction $A' + B'$ to be P . It is clear that our (qualified) general rule for forming disjunctions demonstrates the feasibility of the idempotence and commutation rules (as in the second and fourth claims of (2.2.1.5) *and* in the first and third claims of (2.2.1.6) in Chapter I).

To form the disjunction of three or more propositions we take a pair of them and apply the above rule (for the disjunction of a pair of propositions) to this pair to form a single proposition and continue in this way till we are left with a single proposition representing the disjunction of them all. We clearly always finish up with a proposition which is the disjunction of all the projections of the propositions moved up or down a certain distance. This distance can depend on the order in which we form pairs of propositions but the shape of the region representing the disjunction of them all will always be the same, and the result of pairing in one way will always lie directly above or below (or in the same plane as) the result of pairing in another way. So the association rule for disjunctions will hold in the sense of equivalence, and this demonstrates the feasibility of the sixth claim in (2.2.1.5) of Chapter I.

We say that propositions are ‘mutually exclusive’ when their projections on the home plane are mutually exclusive in the usual sense.

If propositions A' , B' and C' are mutually exclusive but not exhaustive and are at distances α , β and γ below the home plane, then, by (I.8) we have for the distance λ of $(A' + B') + C'$ below the home plane the formula

$$\lambda = \{ \{ \alpha, \beta; w_A, w_B \}, \gamma; w_{A+B}, w_C \} \quad (I.9)$$

But because A' , B' and C' are mutually exclusive but not exhaustive the weights w_A , w_B and w_C will be different and ordered, and the proposition depth finally selected will be the one associated with the largest weight. Or if A' , B' and C' are mutually exclusive *and exhaustive* the proposition depth finally selected will necessarily be zero. In any event the result is the same regardless of the order in which we pair off the propositions. We have thus shown the feasibility of the fifth of (2.2.1.6) of Chapter I.

Finally we note (as is easily demonstrated) the feasibility also of the *Constancy of the phase of implication between disjunctions of similarly equivalent but not exhaustive propositions* claimed in section 2.2.1 of Chapter I.

The conjunction of propositions

Any two propositions A and B that are *not* mutually exclusive, and therefore overlap in the home plane, have a 'classical conjunction' which we write as AB and which is defined in the usual way and is therefore represented by the area of overlap of A and B in the home plane. The characteristic value $c(AB)$ of AB is accordingly zero. The conjunction $A'B'$ of any two propositions A' and B' is that of their projections A and B in the home plane (i.e. the conjunction AB) moved down a distance $\alpha + \beta$, α and β being the displacements of A' and B' from A and B as shown in Figure I-4.

It is evident in Figure I-4 that $\alpha + \beta = c(A'B')$, $\alpha = c(A')$ and $\beta = c(B')$. From

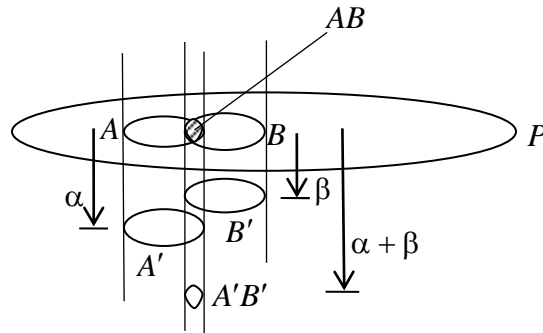


Figure I-4

which we derive

$$c(A'B') = c(A') + c(B'). \quad (\text{I.10})$$

So (I.10) is a general rule applying to any two propositions A' and B' that are not mutually exclusive.

Under this model definition of conjunction we clearly have

$$A'B' \overset{0}{\Leftrightarrow} B'A'$$

as in the second of (2.2.1.6) of Chapter I. And if A , B and C overlap each other, we also evidently have

$$A'(B'C') \overset{0}{\Leftrightarrow} (A'B')C'$$

because, by (I.10), the difference in the drops of $A'(B'C')$ and $(A'B')C'$ from the home plane is

$$\begin{aligned} c(A'(B'C')) - c((A'B')C') &= c(A') + c(B'C') - (c(A'B') + c(C')) \\ &= c(A') + c(B') + c(C') - (c(A') + c(B') + c(C')) = 0 \end{aligned}$$

Hence, by rule (I.4), the fourth claim of (2.2.1.6) of Chapter I is justified.

We clearly have also, by repeated application of (I-10), the general rule

$$c(A'B'...) = c(A') + c(B') + \dots \quad (\text{I.11})$$

for the characteristic value of the conjunction of any number of propositions whose projections on the home plane overlap one another.

From the general rule (I.4) for phases of implication we can justify the first claim in (2.2.1.7) of Chapter I to the effect that if $A' \Rightarrow^\alpha C'$ and $B' \Rightarrow^\beta D'$, and A and B overlap, then $A'B' \Rightarrow^{\alpha+\beta} C'D'$ because

$$c(C'D') - c(A'B') = c(C') + c(D') - (c(A') + c(B')) = c(C') - c(A') + c(D') - c(B') = \alpha + \beta.$$

Also,

$$\text{If } A' \Rightarrow Y' \text{ then, in } A' \overset{-k}{\Leftrightarrow} A'Y', \text{ we have } k = c(Y'), \quad (\text{I.12})$$

because

$$k = c(A'Y') - c(A') = c(A') + c(Y') - c(A') = c(Y').$$

Since, for any propositions A' and Y' we have $A'Y' \Rightarrow A'$, it must be that

$$\text{In } A'Y' \Rightarrow^{-k} A' \text{ we have } k = c(Y'), \quad (\text{I.13})$$

because

$$-k = c(A') - c(A'Y') = c(A') - (c(A') + c(Y')) = -c(Y').$$

Finally we note here the general rule (which follows from (I.4)) relating to any pair of equivalent propositions like A' and A'' in Figure I-2:

$$\text{If } A' \stackrel{-\lambda}{\Leftrightarrow} A'' \text{ then } \lambda = c(A'') - c(A'). \quad (\text{I.14})$$

But of course the converse is not generally true, i.e. given $c(B') - c(A') = \lambda$, it does not follow that A' and B' are equivalent and that $A' \stackrel{-\lambda}{\Leftrightarrow} B'$.

Negation

The negation \bar{A} of any proposition A in the home plane is taken, in the classical way, to be represented by the area between A and P in the home plane. The negation \bar{A}' of any proposition A' equivalent to A but with a (positive or negative) displacement μ below A , is taken to be represented by the area \bar{A} in the home plane displaced vertically a distance $-\mu$. So A' and its negation \bar{A}' are either both in the home plane, or, on opposite sides of and equidistant from the home plane. And clearly

$$\bar{\bar{A}}' \stackrel{0}{\Leftrightarrow} A' \quad (\text{I.15})$$

as claimed in (2.2.1.6) of Chapter I.

Since A and \bar{A} fill region P we have:

$$A' + \bar{A}' \stackrel{0}{\Leftrightarrow} P \quad (\text{I.16})$$

The general duality rules in (2.2.1.5) of Chapter I are clearly reflected in our Venn diagram model on account of the fact that negations, disjunctions and conjunctions of propositions are always *equivalent* to the negations, disjunctions and conjunctions of their projections on the home plane.

Since A' and \bar{A}' are equidistance from and on either side of the home plane we always have that

$$c(\bar{A}') = -c(A') \quad (\text{I.17})$$

Identification of the phase characteristic of knowledge with the characteristic values of the associated propositions

Not all propositions in our Venn diagram represent possible states of *knowledge* (pure or otherwise) even though they may be logically legitimate claims. A proposition (proposed by us at a certain time) might for example, claim incompatible properties and not qualify as a possible state of knowledge on that account. So, not all propositions in our Venn diagram have characteristic *phases* even though they do have characteristic *values*. Nonetheless, by means of the identification

$$\text{ch}(Y') = c(Y') \tag{I.18}$$

which we suppose applies whenever Y' *could* represent a state of knowledge, the claims made (in the main text) regarding phases characteristic of knowledge will be seen to be feasible.

Suppose for example that $Y' \overset{-\lambda}{\Leftarrow} \overset{\lambda}{\Rightarrow} Y''$ then we have, by (I.14) that

$$c(Y'') = c(Y') + \lambda$$

and if Y' (and therefore Y'') represent possible states of knowledge we have, by (I.18), that

$$\text{ch}(Y'') = \text{ch}(Y') + \lambda \tag{I.19}$$

in agreement with *the second addition rule for phases characteristic of knowledge* derived at the beginning of section 1 of Chapter II.

If knowledge A' is compatible with knowledge B' , and states of knowledge A' and B' are compatible with knowledge C' etc, then we could hold the combined knowledge $A'B'...$ and by the identification (I.18)

$$\text{ch}(A'B'...) = c(A'B'...), \quad \text{ch}(A') = c(A'), \quad \text{ch}(B') = c(B'), \dots$$

But by (I.11)

$$c(A'B'...) = c(A') + c(B') + \dots$$

so we arrive at

$$\text{ch}(A'B'...) = \text{ch}(A') + \text{ch}(B') + \dots \tag{I.20}$$

which shows the feasibility of *the first addition rule for phases characteristic of knowledge* claimed in section 2.4 of Chapter I.

In a similar manner we can show from (I.12) and (I.13) the feasibility of the claims made in (2.2.1.20) and (2.2.1.21) of Chapter I. For example, in $A'Y' \Rightarrow^{-k} A'$

where Y' represents a possible state of knowledge, we have, by (I.13) that $k = c(Y')$ and using (I.18)

$$k = \text{ch}(Y')$$

as claimed in (2.2.1.21).

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