The Kramers-Wigner Theorem: Time-Reversal Invariance, Antiunitary Operators, and Degeneracy in Fermionic Systems

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Abstract

This monograph provides a systematic treatment of Kramers degeneracy, investigating its deep-rooted origins within the framework of space-time symmetries in quantum mechanics. The investigation focuses on the nature of the time-reversal operator, exploring the mathematical peculiarities associated with antiunitary transformations and their fundamental distinction from conventional unitary symmetries

Contents

1 Parity symmetry

Parity is spatial inversion. For example, in the one-dimensional case it is the transformation $x \to -x$, while in the three-dimensional case:

$$(x, y, z) \longrightarrow (x', y', z')$$

The transformation equations:

$$x' = -x, \; y' = -y, \; z' = -z \tag{1}$$

The transformation matrix:

$$R^{(parity)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{2}$$

which is an orthogonal matrix with $\det R = -1$. It clearly follows that (1) is not a continuous transformation, i.e., reducible by continuity to the identical transformation. We will therefore say that parity is a *discrete transformation*. In the framework of quantum mechanics, it is preferable to act on the state kets rather than on the coordinate system [1]. Without loss of generality, consider a quantum system consisting of a spinless, non-relativistic particle. If $\mathcal{H}$ is the Hilbert space associated with the system, given the state $|\psi\rangle \in \mathcal{H}$, the spatially inverted state is $\widehat{\mathcal{P}}\,|\psi\rangle$ where $\widehat{\mathcal{P}}$ is the *parity operator*, which we assume to be unitary. In other words, we have the transformation:

$$|\psi\rangle \longrightarrow \widehat{\mathcal{P}}\,|\psi\rangle$$

Denoting by $\hat{\mathbf{x}}$ the Hermitian operator corresponding to the observable position $\mathbf{x}$, our request is:

$$\left\langle \psi|\widehat{\mathcal{P}}^{\dagger}\hat{\mathbf{x}}\widehat{\mathcal{P}}|\psi \right\rangle = -\left\langle \psi|\hat{\mathbf{x}}|\psi\right\rangle, \quad \forall\,|\psi\rangle \in \mathcal{H} \tag{3}$$

In other words, spatial inversion causes the sign of the expectation value of the position observable to be inverted.

Lemma 1 *Parity anticommutes with position*

$$\left\{\widehat{\mathcal{P}},\hat{\mathbf{x}}\right\} = 0 \tag{4}$$

Proof. Taking into account the unity of $\widehat{\mathcal{P}}$:

$$\widehat{\mathcal{P}}^{\dagger}\hat{\mathbf{x}}\widehat{\mathcal{P}} = -\hat{\mathbf{x}} \Longrightarrow \underbrace{\widehat{\mathcal{P}}\widehat{\mathcal{P}}^{\dagger}}_{=\hat{1}}\hat{\mathbf{x}}\widehat{\mathcal{P}} = -\widehat{\mathcal{P}}\hat{\mathbf{x}} \Longleftrightarrow \hat{\mathbf{x}}\widehat{\mathcal{P}} = -\widehat{\mathcal{P}}\hat{\mathbf{x}} \Longleftrightarrow \left\{\widehat{\mathcal{P}},\hat{\mathbf{x}}\right\} = 0 \tag{5}$$

■

We have seen how $\widehat{\mathcal{P}}$ operates on the state kets $|\psi\rangle$; now let's see how it operates on the position eigenkets $|\mathbf{x}\rangle$.

Theorem 1

$$\widehat{\mathcal{P}}\,|\mathbf{x}\rangle = e^{i\varphi}\,|-\mathbf{x}\rangle\,, \quad \varphi \in \mathbb{R} \tag{6}$$

Proof.

$$\left(\hat{\mathbf{x}}\widehat{\mathcal{P}}\right)|\mathbf{x}\rangle \underset{\text{eq. (4)}}{=} \left(-\widehat{\mathcal{P}}\hat{\mathbf{x}}\right)|\mathbf{x}\rangle = -\widehat{\mathcal{P}}\left(\hat{\mathbf{x}}\,|\mathbf{x}\rangle\right) = -\hat{\mathbf{x}}\left(\widehat{\mathcal{P}}\,|\mathbf{x}\rangle\right)$$

i.e. $\widehat{\mathcal{P}}\,|\mathbf{x}\rangle$ is an eigenket of $\hat{\mathbf{x}}$ with eigenvalue $-\mathbf{x}$. Since the spectrum $\sigma(\hat{\mathbf{x}})$ is nondegenerate, the eigenket system $\left\{|-\mathbf{x}\rangle\,,\widehat{\mathcal{P}}\,|\mathbf{x}\rangle\right\}$ is linearly dependent. It follows:

$$\exists c \in \mathbb{C} \mid \widehat{\mathcal{P}}\,|\mathbf{x}\rangle = c\,|-\mathbf{x}\rangle$$

In polar representation $c = |c|\,e^{i\varphi}$; the unitarity of $\widehat{\mathcal{P}}$ implies $|c| = 1$, hence the statement. ■

Since a constant phase factor is unobservable, we set $\varphi = 0$:

$$\widehat{\mathcal{P}}\,|\mathbf{x}\rangle = |-\mathbf{x}\rangle \tag{7}$$

This relation implies that $\widehat{\mathcal{P}}$ is Hermitian. Ultimately, $\widehat{\mathcal{P}}$ is Hermitian and unitary:

$$\widehat{\mathcal{P}}^{-1} = \widehat{\mathcal{P}}^{\dagger} = \widehat{\mathcal{P}}$$

By a well-known property, the spectrum of this operator is $\sigma\left(\widehat{\mathcal{P}}\right) \equiv \sigma_d\left(\widehat{\mathcal{P}}\right) = \{-1,+1\}$.

We have established (Teorema ()) that parity anticommutes with position. Let us now study the behavior of the observable linear momentum with respect to parity. In classical mechanics:

$$\mathbf{p} = m\frac{d\mathbf{x}}{dt} \underset{\mathbf{x}\to-\mathbf{x}}{\longrightarrow} m\frac{d(-\mathbf{x})}{dt} = -m\frac{d\mathbf{x}}{dt} = -\mathbf{p}$$

That is, in classical mechanics, linear momentum is odd with respect to parity. In quantum mechanics, we must argue in terms of infinitesimal translations, since linear momentum is the generator of translations. The infinitesimal translation operator acts on the eigenkets of position in the following way: $\hat{\tau}(d\mathbf{x})|\mathbf{x}\rangle = |\mathbf{x}+d\mathbf{x}\rangle$ with [1]:

$$\hat{\tau}(d\mathbf{x}) = \hat{1} - \frac{i}{\hbar}\hat{\mathbf{p}}\cdot d\mathbf{x} \tag{8}$$

Lemma 2

$$\left\{\widehat{\mathcal{P}}, \hat{\mathbf{p}}\right\} = 0 \tag{9}$$

Proof.

$$\left(\widehat{\mathcal{P}}\hat{\tau}(d\mathbf{x})\right)|\mathbf{x}\rangle = \widehat{\mathcal{P}}|\mathbf{x}+d\mathbf{x}\rangle = |-(\mathbf{x}+d\mathbf{x})\rangle$$
$$\left(\hat{\tau}(-d\mathbf{x})\widehat{\mathcal{P}}\right)|\mathbf{x}\rangle = \hat{\tau}(-d\mathbf{x})|-\mathbf{x}\rangle = |-(\mathbf{x}+d\mathbf{x})\rangle$$

It follows, taking into account the completeness of the autokets system of the position$\{|\mathbf{x}\rangle\}$:

$$\widehat{\mathcal{P}}\hat{\tau}(d\mathbf{x}) = \hat{\tau}(-d\mathbf{x})\widehat{\mathcal{P}} \Longleftrightarrow \widehat{\mathcal{P}}\left(\hat{1} - \frac{i}{\hbar}\hat{\mathbf{p}}\cdot d\mathbf{x}\right) = \left(\hat{1} + \frac{i}{\hbar}\hat{\mathbf{p}}\cdot d\mathbf{x}\right)\widehat{\mathcal{P}}$$
$$\Longleftrightarrow \widehat{\mathcal{P}} - \frac{i}{\hbar}\widehat{\mathcal{P}}(\hat{\mathbf{p}}\cdot d\mathbf{x}) = \widehat{\mathcal{P}} + \frac{i}{\hbar}(\hat{\mathbf{p}}\cdot d\mathbf{x})\widehat{\mathcal{P}} \Longleftrightarrow \widehat{\mathcal{P}}(\hat{\mathbf{p}}\cdot d\mathbf{x}) = -(\hat{\mathbf{p}}\cdot d\mathbf{x})\widehat{\mathcal{P}},\ \forall d\mathbf{x}$$

from which the assertion. ■

Theorem 2

$$\widehat{\mathcal{P}}|\mathbf{p}\rangle = e^{i\varphi}|-\mathbf{p}\rangle, \quad \varphi \in \mathbb{R} \tag{10}$$

Proof.

$$\left(\hat{\mathbf{p}}\widehat{\mathcal{P}}\right)|\mathbf{x}\rangle \underset{\text{eq. (9)}}{=} \left(-\widehat{\mathcal{P}}\hat{\mathbf{p}}\right)|\mathbf{p}\rangle = -\widehat{\mathcal{P}}(\hat{\mathbf{p}}|\mathbf{p}\rangle) = -\hat{\mathbf{p}}\left(\widehat{\mathcal{P}}|\mathbf{p}\rangle\right)$$

i.e. $\widehat{\mathcal{P}}|\mathbf{p}\rangle$ is an eigenket of $\hat{\mathbf{p}}$ with eigenvalue $-\mathbf{p}$. Since the spectrum $\sigma(\hat{\mathbf{p}})$ is nondegenerate, the eigenket system $\left\{|-\mathbf{p}\rangle, \widehat{\mathcal{P}}|\mathbf{p}\rangle\right\}$ is linearly dependent. It follows:

$$\exists c \in \mathbb{C} \mid \widehat{\mathcal{P}}|\mathbf{p}\rangle = c|-\mathbf{p}\rangle$$

In polar representation $c = |c|\,e^{i\varphi}$; the unitarity of P implies $|c| = 1$, hence the statement. ■

Since a constant phase factor is unobservable, we set $\varphi = 0$:

$$\widehat{\mathcal{P}}|\mathbf{p}\rangle = |-\mathbf{p}\rangle \tag{11}$$

Conclusion 1 *The position and linear momentum observables are odd under parity.*

Let's move on to angular momentum. For orbital angular momentum, we proceed classically:

$$\mathbf{L} = \mathbf{x}\wedge\mathbf{p}$$

By the conclusion (1), $\mathbf{L}$ is even by parity or what is the same:

$$\left[\widehat{\mathcal{P}}, \mathbf{L}\right] = 0 \tag{12}$$

On the other hand, in the framework of the orthogonal group O(3), we have seen that the matrix that realizes the spatial inversion is the (2).

$$R^{(parity)}R^{(rot)} = R^{(rot)}R^{(parity)}, \quad \forall R^{(rot)} \in SO(3) \tag{13}$$

that is, any rotation followed by a spatial inversion is equivalent to a spatial inversion followed by rotation.

Notation 3 *In (13) $SO(3)$ is the group of unimodular orthogonal matrices 3×3 ($\det R = +1$).*

The next step is to consider the quantum observable total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$ as the generator of rotations. A rotation by an angle ϕ around an oriented direction of unit vector $\mathbf{n}$ corresponds to a rotation of the state ket $|\psi\rangle \in \mathcal{H}$. For infinitesimal rotations [1]:

$$\widehat{\mathcal{D}}(\mathbf{n}, d\phi) = \hat{1} - \frac{i}{\hbar}\hat{\mathbf{J}} \cdot \mathbf{n} d\phi \tag{14}$$

where $\hat{\mathbf{J}} = \left(\hat{J}_x, \hat{J}_y, \hat{J}_z\right)$ is the Hermitian operator corresponding to the observable $\mathbf{J}$. Eq. (13) suggests:

$$\widehat{\mathcal{P}}\widehat{\mathcal{D}}(\mathbf{n}, d\phi) = \widehat{\mathcal{D}}(\mathbf{n}, d\phi)\widehat{\mathcal{P}}, \quad \forall \mathbf{n} \in \mathbb{R}^3 \tag{15}$$

That is

$$\widehat{\mathcal{P}}\left(\hat{1} - \frac{i}{\hbar}\hat{\mathbf{J}} \cdot \mathbf{n} d\phi\right) = \left(\hat{1} - \frac{i}{\hbar}\hat{\mathbf{J}} \cdot \mathbf{n} d\phi\right)\widehat{\mathcal{P}}$$

$$-\frac{i}{\hbar}\hat{\mathbf{J}} \cdot \mathbf{n} d\phi = -\frac{i}{\hbar}\hat{\mathbf{J}} \cdot \mathbf{n} d\phi\widehat{\mathcal{P}}$$

$\hat{J}_n \equiv \hat{\mathbf{J}} \cdot \mathbf{n}$

$$\widehat{\mathcal{P}}\hat{J}_n = \hat{J}_n\widehat{\mathcal{P}}, \ \forall \mathbf{n} \in \mathbb{R}^3$$

i.e.

$$\left[\widehat{\mathcal{P}}, \hat{\mathbf{J}}\right] = 0 \tag{16}$$

Conclusion 2 *The observable total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is even under parity.*

In particular $\mathbf{L}$ and $\mathbf{S}$ are even under parity.

Definition 1 *Odd vectors by parity are called* **polar vectors**. *Even vectors by parity are called* **axial vectors** *o* **pseudovectors** .

So $\mathbf{x}, \mathbf{p}$ are polar vectors, while $\mathbf{J}, \mathbf{L}, \mathbf{S}$ are axial vectors. From vector calculus we know that the dot product of two vectors is a scalar, i.e., invariant under space inversion:

$$\mathbf{a} \cdot \mathbf{b} \underset{\text{sp. inv.}}{\longrightarrow} (-\mathbf{a}) \cdot (-\mathbf{b}) = \mathbf{a} \cdot \mathbf{b}, \ \forall \mathbf{a}, \mathbf{b} \in \mathbb{R}^3$$

This is an intuitive result because a number doesn't change sign if we reverse the orientation of the Cartesian axes. In our formalism, we have that $\mathbf{x} \cdot \mathbf{p}$ è pari per parità. is even by parity. Note that we have performed the scalar product of two polar vectors. Conversely, we expect an odd result by parity if we multiply an axial vector by a polar vector. For example $\mathbf{S} \cdot \mathbf{x}$. In fact:

$$\left[\widehat{\mathcal{P}}, \hat{\mathbf{S}}\right] = 0, \ \left\{\widehat{\mathcal{P}}, \hat{\mathbf{x}}\right\} = 0$$

It follows

$$\left(\hat{\mathbf{S}} \cdot \hat{\mathbf{x}}\right)\widehat{\mathcal{P}} = \hat{\mathbf{S}} \cdot \left(\hat{\mathbf{x}}\widehat{\mathcal{P}}\right) = -\hat{\mathbf{S}} \cdot \left(\widehat{\mathcal{P}}\hat{\mathbf{x}}\right) = -\left(\hat{\mathbf{S}}\widehat{\mathcal{P}}\right) \cdot \hat{\mathbf{x}} = -\widehat{\mathcal{P}}\left(\hat{\mathbf{S}} \cdot \hat{\mathbf{x}}\right)$$

$$\Longrightarrow \left\{\widehat{\mathcal{P}}, \hat{\mathbf{S}} \cdot \hat{\mathbf{x}}\right\} = 0$$

while for any scalar operator $\hat{A}$: $\left[\widehat{\mathcal{P}}, \hat{A}\right] = 0$. This behavior is expressed by saying that $\mathbf{S} \cdot \mathbf{x}$ is a pseudoscalar, as is $\mathbf{L} \cdot \mathbf{x}$ and $\mathbf{J} \cdot \mathbf{x}$. So:

$$(\text{polar vector}) \cdot (\text{axial vector}) = \text{pseudoscalar}$$

Obviously:

$$(\text{axial vector}) \cdot (\text{axial vector}) = \text{scalar}$$

such as, $\mathbf{L} \cdot \mathbf{S}$.

1.1 Violation of parity

As established in the previous issue, in quantum mechanics parity is a Hermitian operator, so one might ask whether it represents an observable. The answer is affirmative, and it follows that this observable is a constant of motion for a conservative system if $\left[\hat{H}, \widehat{\mathcal{P}}\right] = 0$, where $\hat{H}$ is the Hamiltonian of the quantum system. Considering spatial inversion to be a universal symmetry operation, we expect that, no matter what quantum system we consider, $\left[\hat{H}, \widehat{\mathcal{P}}\right] = 0$. This assertion was refuted in 1956 by a famous experiment based on β decay, which, among other things, proved a conjecture of T.L. Lee and C.N. Yang [2].

2 Time reversal symmetry

In addition to the spatial inversion $\mathbf{x} \to -\mathbf{x}$, we can consider the *time reversal* $t \to -t$. This is a well-defined operation in classical mechanics, but problematic in quantum mechanics. Indeed, in the latter case, while the position $\mathbf{x}$ is an observable, the time t is a real parameter. On the other hand, the transformation $t \to -t$ determines an exchange of the future with the past, so the appropriate term is *inversion of motion*. Without loss of generality, let us consider a mechanical system consisting of a single non-relativistic particle. In the Hamiltonian formulation, the differential equations of motion (*Hamilton equations*), with the appropriate initial conditions, are:

$$\dot{\mathbf{x}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{x}} \tag{17}$$
$$\mathbf{x}(0) = \mathbf{x}_0, \quad \mathbf{p}(0) = \mathbf{p}_0$$

where $H(\mathbf{x}, \mathbf{p}, t)$ is the hamiltonian. Solving (17) yields the time equation of motion $\mathbf{x} = \mathbf{x}(t), \ \forall t \in [0, +\infty)$. By performing time reversal, i.e., the inversion of motion, we move from $\mathbf{x}(t)$ to $\mathbf{x}(-t)$. If the function $\mathbf{x}(-t)$ solves the problem (17) we say that the dynamics of the system is time-reversal invariant. This is clearly true if the Hamiltonian does not explicitly depend on time (a conservative system). Conversely, in the presence of dissipative or velocity-dependent forces (such as the Lorentz force due to a magnetic field), the dynamical evolution of the system is not time-reversal invariant.

Let's move on to quantum mechanics. For a spinless particle in a conservative field of potential energy V(x), the dynamical evolution of the system is governed by the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V\right)\psi \tag{18}$$

If $\psi(\mathbf{x}, -t)$ is a solution of (18), we check whether $\phi(\mathbf{x}, t) \equiv \psi(\mathbf{x}, -t)$ is also a solution. We get:

$$\frac{\partial}{\partial t}\psi(\mathbf{x}, -t) \underset{t'=-t}{=} \frac{\partial \psi(\mathbf{x}, t')}{\partial t'} \underbrace{\frac{dt'}{dt}}_{=-1} = -\frac{\partial \psi(\mathbf{x}, t')}{\partial t'}$$

So the first member of (18) becomes:

$$i\hbar \frac{\partial \phi(\mathbf{x}, t)}{\partial t} = -i\hbar \frac{\partial \psi(\mathbf{x}, t')}{\partial t'} \tag{19}$$

The second member transforms as:

$$\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V\right)\phi(\mathbf{x}, t) = \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V\right)\psi(\mathbf{x}, t') \tag{20}$$

By (19) and (20) it follows that $\phi(\mathbf{x}, t) \equiv \psi(\mathbf{x}, -t)$ is not a solution. Incidentally:

Proposition 1 *If $\psi(\mathbf{x}, t)$ is a solution of (18), the complex conjugate function $\psi^*(\mathbf{x}, t)$ is also a solution.*

Proof. Let's take the complex conjugate of the (18):

$$i\hbar\frac{\partial\psi^*}{\partial t} = \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V\right)\psi^* \tag{21}$$

$t \to -t \Longrightarrow \frac{\partial}{\partial t} \to -\frac{\partial}{\partial(-t)}$, so

$$\begin{aligned}
-i\hbar\frac{\partial\psi^*(x,-t)}{\partial(-t)} &= \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V\right)\psi^*(x,-t)\\
i\hbar\frac{\partial\psi^*(x,-t)}{\partial t} &= \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V\right)\psi^*(x,-t)
\end{aligned}$$

■

From the proposition just proved, it follows that time reversal is somehow related to complex conjugation.

2.1 Digression on symmetry operations

Let $\mathcal{H}$ denote the Hilbert space associated with a nonrelativistic quantum system S_q. Rotations/translations in physical space correspond to unitary transformations in $\mathcal{H}$. Space inversion is also described by a unitary transformation. In general, a unitary transformation preserves the norm of the vectors in $\mathcal{H}$ and therefore, the scalar product. In symbols:

$$|\psi\rangle \to \left|\tilde{\psi}\right\rangle, \quad |\phi\rangle \to \left|\tilde{\phi}\right\rangle$$

where

$$\left|\tilde{\psi}\right\rangle = \hat{U}|\psi\rangle, \quad \left|\tilde{\phi}\right\rangle = \hat{U}|\phi\rangle, \qquad \hat{U} = \text{unitary operator}$$

It follows

$$\left\langle\tilde{\psi}|\tilde{\phi}\right\rangle = \left\langle\psi|\hat{U}^\dagger\hat{U}|\phi\right\rangle \underset{\hat{U}^\dagger\hat{U}=\hat{1}}{=} \langle\psi|\phi\rangle, \quad \forall|\psi\rangle, |\phi\rangle \in \mathcal{H} \tag{22}$$

Intuitively, if $|\psi\rangle$ and $|\phi\rangle$ are rotated by the same angle, the scalar product $\langle\psi|\phi\rangle$ remains unchanged. Therefore, the invariance of the scalar product is essential for a transformation to be a symmetry transformation. However, we have established that time reversal is related to complex conjugation. This circumstance suggests replacing the requirement (22) with

$$\left\langle\tilde{\psi}|\tilde{\phi}\right\rangle = \langle\psi|\phi\rangle^*, \quad \forall|\psi\rangle, |\phi\rangle \in \mathcal{H} \tag{23}$$

Definition 2 *In a Hilbert space $\mathcal{H}$ a transformation is said to be* **antiunitary** *if*

$$|\psi\rangle \longrightarrow \left|\tilde{\psi}\right\rangle, \ |\phi\rangle \longrightarrow \left|\tilde{\phi}\right\rangle \Longrightarrow \left\langle\tilde{\phi}|\tilde{\psi}\right\rangle = \langle\psi|\phi\rangle^*, \quad \forall|\psi\rangle, |\phi\rangle \in \mathcal{H} \tag{24}$$

That is, while a unitary transformation returns the same value as the dot product, an antiunitary transformation returns the complex conjugate.

Definition 3 *An operator $\hat{\vartheta}$ is said to be* **antilinear** *if*

$$\hat{\vartheta}(\lambda|\psi\rangle + \mu|\phi\rangle) = \lambda^*\hat{\vartheta}|\psi\rangle + \mu^*\hat{\vartheta}|\phi\rangle, \quad \forall|\psi\rangle, |\phi\rangle \in \mathcal{H}, \ \forall\lambda, \mu \in \mathbb{C} \tag{25}$$

Let us assume that a antiunitary transformation is realized by a special antilinear operator, which we call **antiunitary** . An antiunitary operator is expressed by the product of a unitary operator $\hat{U}$ by a suitable antilinear operator $\hat{K}$:

$$\hat{K}(\lambda |\psi\rangle) = \lambda^* \hat{K} |\psi\rangle , \quad \forall |\psi\rangle \in \mathcal{H}, \ \forall \lambda \in \mathbb{C} \tag{26}$$

If we take as an orthonormal basis of $\mathcal{H}$ the system$\{|a_n\rangle\}$ of eigenkets of some observable A with a purely discrete spectrum:

$$|\psi\rangle = \sum_n |a_n\rangle \langle a_n|\psi\rangle , \quad \forall |\psi\rangle \in \mathcal{H}$$

It follows

$$\hat{K}|\psi\rangle = \hat{K}\sum_n |a_n\rangle \langle a_n|\psi\rangle = \sum_n \hat{K}|a_n\rangle \langle a_n|\psi\rangle = \sum_n \hat{K}(\langle a_n|\psi\rangle |a_n\rangle) = \sum_n \langle a_n|\psi\rangle^* \hat{K}|a_n\rangle$$

The antilinear operator $\hat{K}$ is such that

$$\hat{K}|a_n\rangle = |a_n\rangle , \quad \forall n$$

i.e. leave the basic kets unchanged or what is the same, every eigenket of A is an eigenket of $\hat{K}$ with eigenvalue 1. It follows

$$|\psi\rangle = \sum_n |a_n\rangle \langle a_n|\psi\rangle \Longrightarrow \hat{K}|\psi\rangle = \sum_n \hat{K} a_n \langle a_n|\psi\rangle^* , \quad \forall |\psi\rangle \in \mathcal{H} \tag{27}$$

$\hat{\theta} = \hat{U}\hat{K}$ is antilinear, where $\hat{U}$ is any unitary operator and $\hat{K}$ is defined by (27). In fact:

$$\begin{aligned}\hat{\theta}(\lambda|\psi\rangle + \mu|\phi\rangle) &= \hat{U}\hat{K}(\lambda|\psi\rangle + \mu|\phi\rangle) = \hat{U}\left[\hat{K}(\lambda|\psi\rangle) + \hat{K}(\mu|\phi\rangle)\right] \\ &= \hat{U}\left(\lambda^*\hat{K}|\psi\rangle + \mu^*\hat{K}|\phi\rangle\right) = \lambda^*\hat{\theta}|\psi\rangle + \mu^*\hat{\theta}|\phi\rangle ,\end{aligned}$$

Now we have to show that if

$$\left|\tilde{\psi}\right\rangle = \hat{\theta}|\psi\rangle , \quad \left|\tilde{\phi}\right\rangle = \hat{\theta}|\phi\rangle$$

then:

$$\left\langle\tilde{\phi}|\tilde{\psi}\right\rangle = \langle\psi|\phi\rangle^* , \quad \forall |\psi\rangle , |\phi\rangle \in \mathcal{H}$$

With the usual base $\{|a_n\rangle\}$:

$$\begin{aligned}|\psi\rangle &= \sum_n |a_n\rangle \langle a_n|\psi\rangle , \ |\phi\rangle = \sum_n |a_n\rangle \langle a_n|\phi\rangle \\ \left|\tilde{\psi}\right\rangle &= \hat{U}\hat{K}\sum_n |a_n\rangle \langle a_n|\psi\rangle = \sum_n \left(\hat{U}\hat{K}\right)|a_n\rangle \langle a_n|\psi\rangle = \sum_n \left(\hat{U}\hat{K}\right)(\langle a_n|\psi\rangle |a_n\rangle) \\ &= \sum_n \langle a_n|\psi\rangle^* \hat{U}\left(\hat{K}|a_n\rangle\right)\end{aligned}$$

But $\hat{K}|a_n\rangle = |a_n\rangle$

$$\left|\tilde{\psi}\right\rangle = \sum_n \langle\psi|a_n\rangle \hat{U}|a_n\rangle \tag{28}$$

Furthermore

$$\left|\tilde{\phi}\right\rangle = \sum_n \langle\phi|a_n\rangle \hat{U}|a_n\rangle \overset{\text{DC}}{\longleftrightarrow} \left\langle\tilde{\phi}\right| = \sum_n \langle a_n|\phi\rangle \langle a_n| \hat{U}^\dagger$$

where DC stands for "dual correspondence".

$$\left\langle \tilde{\phi} | \tilde{\psi} \right\rangle = \left[\sum_n \langle a_n | \phi \rangle \langle a_n | \hat{U}^\dagger \right] \cdot \left[\sum_{n'} \langle \psi | a_{n'} \rangle \hat{U} | a_{n'} \rangle \right]$$

$$= \sum_n \sum_{n'} \langle a_n | \phi \rangle \underbrace{\left\langle a_n | \overbrace{\hat{U}^\dagger \hat{U}}^{\hat{1}} | a_{n'} \right\rangle}_{\delta_{nn'}} \langle \psi | a_{n'} \rangle$$

$$= \sum_n \langle a_n | \phi \rangle \langle a_n | \psi \rangle^* = \langle \phi | \psi \rangle^*$$

2.2 Time reversal operator

After this digression on anti-unitary transformations, we can elaborate a formal theory of time reversal. We denote the time reversal operator by $\hat{\Theta}$ to distinguish it from a generic antiunitary operator $\hat{\theta}$. It follows that if $|\psi\rangle$ is the state of the system, $\hat{\Theta}|\psi\rangle$ is the time-reversed state (or rather, the state of reversed motion). By analogy with classical mechanics, if $|\psi\rangle = |\mathbf{p}\rangle$ that is, if the system is in a momentum eigenstate, we must have (up to an inessential phase factor):

$$\hat{\Theta} |p\rangle = |-\mathbf{p}\rangle \tag{29}$$

Before deriving the properties of the antiunitary operator $\hat{\Theta}$, let us recall that if the Hamiltonian $\hat{H}$ of the particle does not explicitly depend on time, the (unitary) time evolution operator is:

$$\widehat{\mathcal{U}}(t, t_0) = e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} \tag{30}$$

where t_0 is the initial time.

$$|\psi(t)\rangle = \widehat{\mathcal{U}}(t, t_0) |\psi(t_0)\rangle, \quad \forall t \in \mathbb{R}$$

For $t = t_0 + \delta t$ with $\delta t \ll 1$, developing the second member of (30) in a power series truncated to first order:

$$\widehat{\mathcal{U}}(t, \delta t) = \hat{1} - \frac{i}{\hbar} \hat{H} \delta t \tag{31}$$

where $t_0 = 0$. So the time evolution of the initial state $|\psi_0\rangle \equiv |\psi(0)\rangle$ is:

$$|\psi(\delta t)\rangle = \left(\hat{1} - \frac{i}{\hbar} \hat{H} \delta t \right) |\psi_0\rangle$$

Let us imagine applying the operator $\hat{\Theta}$ to the initial state $|\psi_0\rangle$, then making the system evolve according to the Hamiltonian $\hat{H}$. At $t = \delta t$ the state of the system is

$$\left(\hat{1} - \frac{i}{\hbar} \hat{H} \delta t \right) \hat{\Theta} |\psi_0\rangle \tag{32}$$

i.e. the time evolution at $t = \delta t$ of the time-reversed initial state. Let us now consider the state:

$$\hat{\Theta} |\psi(-\delta t)\rangle \tag{33}$$

that is, the time-reversed state of the time-evolved state at $t = -\delta t$ of the initial state $|\psi_0\rangle$. If the dynamical evolution of the system is invariant under time evolution, the two states (32)-(33) coincide up to an inessential phase factor:

$$\left(\hat{1} - \frac{i}{\hbar} \hat{H} \delta t \right) \hat{\Theta} |\psi_0\rangle = \hat{\Theta} |\psi(-\delta t)\rangle$$

$|\psi(-\delta t)\rangle \underset{\text{eq. (32)}}{=} \left(\hat{1} + \frac{i}{\hbar}\hat{H}\delta t\right)|\psi_0\rangle$, so

$$\begin{aligned}\left(\hat{1} - \frac{i}{\hbar}\hat{H}\delta t\right)\hat{\Theta}|\psi_0\rangle &= \hat{\Theta}\left(\hat{1} + \frac{i}{\hbar}\hat{H}\delta t\right)|\psi_0\rangle \\ \hat{\Theta} - \frac{i}{\hbar}\delta t\hat{H}\hat{\Theta}|\psi_0\rangle &= \hat{\Theta} + \frac{1}{\hbar}\delta t\hat{\Theta}\left(i\hat{H}\right)|\psi_0\rangle \\ -i\hat{H}\hat{\Theta}|\psi_0\rangle &= \hat{\Theta}\left(i\hat{H}\right)|\psi_0\rangle\end{aligned}$$

The initial state can be any: $|\psi_0\rangle \equiv |\eta\rangle\,,\ \forall|\eta\rangle \in \mathcal{H}$, so the following equality holds:

$$-i\hat{H}\hat{\Theta}|\eta\rangle = \hat{\Theta}\left(i\hat{H}\right)|\eta\rangle\,,\ \forall|\eta\rangle \in \mathcal{H} \tag{34}$$

Proposition 2 *If the dynamical evolution of the system is time invariant, the operator $\hat{\Theta}$ in (34) is not unitary.*

Proof. Let's proceed by contradiction: $\hat{\Theta}$ is unitary. So $\hat{\Theta}\left(i\hat{H}\right) = i\hat{\Theta}\hat{H}$; from (34)

$$-i\hat{H}\hat{\Theta}|\eta\rangle = i\hat{\Theta}\hat{H}|\eta\rangle\,,\ \forall|\eta\rangle \in \mathcal{H} \Longrightarrow -\hat{H}\hat{\Theta} = \hat{\Theta}\hat{H}$$

If $|E_n\rangle$ is any self-transfer of energy:

$$\left(\hat{H}\hat{\Theta}\right)|E_n\rangle = -\left(\hat{\Theta}\hat{H}\right)|E_n\rangle = (-E_n)\left(\hat{\Theta}|E_n\rangle\right)$$

i.e. $\hat{\Theta}|E_n\rangle$ is eigenket of the energy with eigenvalue $-E_n$, whatever $E_n > 0$. But this is absurd because the energy spectrum cannot extend from 0 to $-\infty$. ■

From the proposition just proved, it follows that if the system is symmetric under time reversal, we cannot cancel the imaginary unit from (34) The only possible solution is anti-unitarity. $\hat{\Theta}$:

$$\hat{\Theta}\left(i\hat{H}\right)|\eta\rangle = -i\left(\hat{\Theta}\hat{H}\right)|\eta\rangle$$

and by (34)

$$\left[\hat{H}, \hat{\Theta}\right] = 0 \tag{35}$$

Evidently

$$\begin{gathered}\hat{\Theta}\ \text{è antiunitario} \Longrightarrow \exists\hat{V}, \hat{K} \mid \hat{\Theta} = \hat{V}\hat{K} \\ V^\dagger = V^{-1}, \quad \hat{K}|\psi\rangle = \sum_n \hat{K}a_n\langle a_n|\psi\rangle^*\,,\ \forall|\psi\rangle \in \mathcal{H}\end{gathered}$$

$\left|\tilde{\psi}\right\rangle = \hat{\Theta}|\psi\rangle$ is the time-reversed state $|\psi\rangle$. What does represent $\langle\psi|\hat{\Theta}$? The answer is problematic due to a limitation of Dirac notation. This is not surprising because Dirac notation was formulated for linear operators. So an object of the type $\left\langle\phi\left|\hat{\Theta}\right|\psi\right\rangle$ is to be understood $\langle\phi|\cdot\left(\hat{\Theta}|\psi\rangle\right)$:

$$\left\langle\phi\left|\hat{\Theta}\right|\psi\right\rangle = \langle\phi|\cdot\left(\hat{\Theta}|\psi\rangle\right),\ \forall|\psi\rangle, |\phi\rangle \in \mathcal{H}$$

Proposition 3 *However, let's take a linear operator $\hat{X}$,*

$$\left\langle\phi\left|\hat{X}\right|\psi\right\rangle = \left\langle\tilde{\psi}\left|\hat{\Theta}\hat{X}^\dagger\hat{\Theta}^{-1}\right|\tilde{\phi}\right\rangle,\ \forall|\psi\rangle, |\phi\rangle \in \mathcal{H} \tag{36}$$

Proof.

$$|\eta\rangle \stackrel{def}{=} \hat{X}^\dagger |\phi\rangle \Longrightarrow |\eta\rangle \stackrel{\text{CD}}{\leftrightarrow} \langle\phi| \hat{X} \Longrightarrow \left\langle \phi \left| \hat{X} \right| \psi \right\rangle = \left(\langle\phi| \hat{X} \right) \cdot |\psi\rangle = \langle\eta|\psi\rangle$$
$$= \left\langle \tilde{\eta}|\tilde{\psi} \right\rangle^* = \left\langle \tilde{\psi}|\hat{\Theta}\hat{X}^\dagger|\phi \right\rangle = \left\langle \tilde{\psi}|\hat{\Theta}\hat{X}^\dagger\hat{\Theta}^{-1}\hat{\Theta}|\phi \right\rangle = \left\langle \tilde{\psi}|\hat{\Theta}\hat{X}^\dagger\hat{\Theta}^{-1}|\tilde{\phi} \right\rangle$$

■

In the special case of a Hermitian operator $\hat{A}$:

$$\left\langle \phi \left| \hat{A} \right| \psi \right\rangle = \left\langle \tilde{\psi} \left| \hat{\Theta}\hat{A}\hat{\Theta}^{-1} \right| \tilde{\phi} \right\rangle, \quad \forall |\psi\rangle, |\phi\rangle \in \mathcal{H} \tag{37}$$

Definition 4 *An observable A is* **even** *by time reversal if $\hat{\Theta}\hat{A}\hat{\Theta}^{-1} = +\hat{A}$. Conversely, it is* **odd** *by time reversal if $\hat{\Theta}\hat{A}\hat{\Theta}^{-1} = -\hat{A}$.*

For an observable with definite parity, the (37) takes the form:

$$\left\langle \phi \left| \hat{A} \right| \psi \right\rangle = \pm \left\langle \tilde{\psi} \left| \hat{A} \right| \tilde{\phi} \right\rangle, \quad \forall |\psi\rangle, |\phi\rangle \in \mathcal{H} \tag{38}$$

or

$$\left\langle \tilde{\phi} \left| \hat{A} \right| \tilde{\psi} \right\rangle = \pm \left\langle \phi \left| \hat{A} \right| \psi \right\rangle, \quad \forall |\psi\rangle, |\phi\rangle \in \mathcal{H} \tag{39}$$

This relation implies a restriction of the phase factor of the matrix elements of A, taken with respect to time-reversed states. In particular:

$$\left\langle \psi \left| \hat{A} \right| \psi \right\rangle = \pm \left\langle \tilde{\psi} \left| \hat{A} \right| \tilde{\psi} \right\rangle, \quad \forall |\psi\rangle \in \mathcal{H} \tag{40}$$

The right-hand side $\left\langle \psi \left| \hat{A} \right| \psi \right\rangle$ is the expectation value $\langle A\rangle_\psi$ of the observable A in the state $|\psi\rangle$, while $\left\langle \tilde{\psi} \left| \hat{A} \right| \tilde{\psi} \right\rangle$ is the expectation value in the time-reversed state. It follows that if A is even under time-reversal:

$$\langle A\rangle_\psi = + \langle A\rangle_{\tilde{\psi}} \tag{41}$$

If A is odd by time reversal:

$$\langle A\rangle_\psi = - \langle A\rangle_{\tilde{\psi}} \tag{42}$$

A case of physical interest is the linear momentum observable $\mathbf{p}$. It is reasonable to assume that this observable is odd under time reversal:

$$\langle\psi|\hat{\mathbf{p}}|\psi\rangle = -\left\langle \tilde{\psi}|\hat{\mathbf{p}}|\tilde{\psi} \right\rangle, \quad \forall |\psi\rangle \in \mathcal{H}$$

equivalent to

$$\hat{\Theta}\hat{\mathbf{p}}\hat{\Theta}^{-1} = -\hat{\mathbf{p}}$$

It follows

$$\left\{ \hat{\Theta}, \hat{\mathbf{p}} \right\} = 0 \tag{43}$$

After a few simple steps and less than one phase:

$$\hat{\Theta} |\mathbf{p}\rangle = |-\mathbf{p}\rangle, \quad \forall \mathbf{p} \in \sigma(\hat{\mathbf{p}}) \tag{44}$$

For the position observable we require parity $(+1)$ for time reversal:

$$\langle\psi|\hat{\mathbf{x}}|\psi\rangle = \left\langle \tilde{\psi}|\hat{\mathbf{x}}|\tilde{\psi} \right\rangle, \quad \forall |\psi\rangle \in \mathcal{H}$$

It follows (except for one phase):

$$\hat{\Theta}\left|\mathbf{x}\right\rangle = \left|\mathbf{x}\right\rangle, \ \ \forall \mathbf{x} \in \sigma\left(\hat{\mathbf{x}}\right) \tag{45}$$

is. any time-reversed position outlet, is still an eigenket of that observable, with the same eigenvalue.

We study the effect of $\hat{\Theta}$ on fundamental commutation relations. In particular:

$$\left[\hat{x}_k, \hat{p}_{k'}\right] = i\hbar\delta_{kk'} \tag{46}$$

More formally $\left[\hat{x}_k, \hat{p}_{k'}\right] = i\hbar\delta_{kk'}\hat{1}$. We have

$$\left[\hat{x}_k, \hat{p}_{k'}\right]\left|\psi\right\rangle = i\hbar\delta_{kk'}\left|\psi\right\rangle, \ \ \forall \left|\psi\right\rangle \in \mathcal{H}$$

We apply $\hat{\Theta}$

$$\hat{\Theta}\left[\hat{x}_k, \hat{p}_{k'}\right]\left(\hat{\Theta}^{-1}\hat{\Theta}\right)\left|\psi\right\rangle = \underbrace{\hat{\Theta}\left(i\hbar\delta_{kk'}\right)\left|\psi\right\rangle}_{=-i\hbar\delta_{kk'}\hat{\Theta}\left|\psi\right\rangle}, \ \ \forall \left|\psi\right\rangle \in \mathcal{H} \tag{47}$$

Let's make it explicit

$$\hat{\Theta}\left[\hat{x}_k, \hat{p}_{k'}\right]\hat{\Theta}^{-1} = \left[\underbrace{\hat{\Theta}\hat{x}_k\hat{\Theta}^{-1}}_{=\hat{x}_k}, \underbrace{\hat{\Theta}\hat{p}_{k'}\hat{\Theta}^{-1}}_{=-\hat{p}_{k'}}\right] = \left[\hat{x}_k, -\hat{p}_{k'}\right]$$

The first member of (47):

$$\hat{\Theta}\left[\hat{x}_k, \hat{p}_{k'}\right]\left(\hat{\Theta}^{-1}\hat{\Theta}\right)\left|\psi\right\rangle = \left[\hat{x}_k - \hat{p}_{k'}\right]\hat{\Theta}\left|\psi\right\rangle$$

which replaced in the (47):

$$\left[\hat{x}_k, -\hat{p}_{k'}\right]\hat{\Theta}\left|\psi\right\rangle = -i\hbar\delta_{kk'}\hat{\Theta}\left|\psi\right\rangle, \ \ \forall \left|\psi\right\rangle \in \mathcal{H}$$

Recall that $\hat{\Theta}\left|\psi\right\rangle$ is the time-reversed state. Ultimately, we have the following scheme:

$$\begin{cases} \left[\hat{x}_k, \hat{p}_{k'}\right]\left|\psi\right\rangle = i\hbar\delta_{kk'}\left|\psi\right\rangle \\ \left[\hat{x}_k, -\hat{p}_{k'}\right]\hat{\Theta}\left|\psi\right\rangle = -i\hbar\delta_{kk'}\hat{\Theta}\left|\psi\right\rangle \end{cases}, \ \ \forall \left|\psi\right\rangle \in \mathcal{H} \tag{48}$$

which shows the time-reversal invariance of the canonical commutation relation (46). This is vital for the Heisenberg uncertainty relation to retain its validity. These considerations can be extended to the angular momentum $\mathbf{J}$, whose components obey the commutation relation:

$$\left[\hat{J}_k, \hat{J}_{k'}\right] = i\hbar\varepsilon_{kk'r}\hat{J}_r \tag{49}$$

with odd $\mathbf{J}$ for time reversal:

$$\hat{\Theta}\hat{\mathbf{J}}\hat{\Theta}^{-1} = -\hat{\mathbf{J}} \tag{50}$$

Since we are considering a spinless particle, $\hat{\mathbf{J}} = \mathbf{L} = \mathbf{x} \wedge \mathbf{p}$, from which the parity (-1) of the observable $\mathbf{J}$ immediately follows.

***

If $|\psi_0\rangle$ is the initial state ($t = 0$) of the quantum system we are studying (spinless particle in a conservative field), in the coordinate basis $\{|\mathbf{x}\rangle\}$:

$$|\psi_0\rangle = \int_{\mathbb{R}^3} d^3x \, |\mathbf{x}\rangle \langle \mathbf{x}|\psi_0\rangle \tag{51}$$

Here $\langle \mathbf{x}|\psi_0\rangle = \psi_0(\mathbf{x})$ i.e. the wave function of the initial state. We apply the time reversal operator to the initial state:

$$\hat{\Theta} |\psi_0\rangle = \int_{\mathbb{R}^3} d^3x \hat{\Theta} |\mathbf{x}\rangle \langle \mathbf{x}|\psi_0\rangle$$

Let's computation

$$\begin{aligned} \hat{\Theta} |\mathbf{x}\rangle \langle \mathbf{x}|\psi_0\rangle &= \hat{\Theta} \left(\langle \mathbf{x}|\psi_0\rangle |\mathbf{x}\rangle \right) = \langle \mathbf{x}|\psi_0\rangle^* \hat{\Theta} |\mathbf{x}\rangle \\ &= \langle \mathbf{x}|\psi_0\rangle^* |\mathbf{x}\rangle = |\mathbf{x}\rangle \langle \mathbf{x}|\psi_0\rangle^* \end{aligned}$$

So

$$\hat{\Theta} |\psi_0\rangle = \int_{\mathbb{R}^3} d^3x \, |\mathbf{x}\rangle \langle \mathbf{x}|\psi_0\rangle^* \tag{52}$$

It follows that the wave function of the time-reversed initial state is the complex conjugate of the wave function of the given state. This confirms the result previously found in the wave mechanics framework.

A non-trivial consequence of time-reversal invariance for a spinless particle is the following theorem:

Theorem 4 ***Hp 1***. *The Hamiltonian $\hat{H}$ of a spinless particle is time-reversal invariant.* ***Hp 2***. *The spectrum $\sigma\left(\hat{H}\right)$ is nondegenerate.*

Th. *The energy eigenfunctions are real up to a phase factor independent of* $\mathbf{x}$.

Proof. Hp 1 $\underset{\text{eq. (35)}}{\Longrightarrow} \left[\hat{H}, \hat{\Theta}\right] = 0$. Let's refer to the purely discrete spectrum $\hat{H} |E_n\rangle = E_n |E_n\rangle$.

$$\hat{H}\hat{\Theta} |E_n\rangle = \hat{\Theta}\hat{H} |E_n\rangle = \hat{\Theta} E_n |E_n\rangle \underset{E_n \in \mathbb{R}}{=} E_n \left(\hat{\Theta} |E_n\rangle\right)$$

i.e. $|E_n\rangle$, $\hat{\Theta} |E_n\rangle$ are eigenkets of $\hat{H}$ with the same eigenvalue E_n.

Hp 2 $\Longrightarrow \exists \lambda \in \mathbb{C} \mid \hat{\Theta} |E_n\rangle = \lambda |E_n\rangle \underset{\langle E_n|E_n\rangle = 1}{\Longrightarrow} |\lambda| = 1 \Longrightarrow \lambda = e^{i\varphi}, \ \varphi \in \mathbb{R}$. So less than one phase

$$\hat{\Theta} |E_n\rangle = |E_n\rangle$$

Moving on to eigenfunctions:

$$\langle \mathbf{x}|E_n\rangle = \left\langle \mathbf{x}|\hat{\Theta}|E_n \right\rangle$$

But as previously established

$$\left\langle \mathbf{x}|\hat{\Theta}|E_n \right\rangle = \left\langle \mathbf{x}|\hat{\Theta}|E_n \right\rangle^*$$

that is, the assertion. ■

If we relax the assumption of nondegeneration, the theorem might not be true. For example, in the case of the free particle, the Hamiltonian $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m}$ is manifestly invariant under time reversal, and furthermore, by commuting with the linear momentum operator, we have that the energy eigenfunctions are plane waves:

$$u_{\mathbf{p}}(\mathbf{x}) = \frac{1}{(2\pi\hbar^3)^{3/2}} e^{\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{p}} \tag{53}$$

The corresponding eigenvalues:

$$E_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m} = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right), \quad E_{\mathbf{p}} \in \sigma\left(\hat{H}\right) = (0, +\infty) \tag{54}$$

The spectrum $\sigma\left(\hat{H}\right)$ exhibits infinite degeneracy because all eigenfunctions (53) corresponding to p of equal magnitude belong to the same eigenvalue $E_{\mathbf{p}}$. Incidentally, the (53) are complex functions of the real variables (x, y, z).

We conclude this section by observing that the shape of $\hat{\Theta}$ depends on the assigned basis. In the x-representation we saw that the action of $\hat{\Theta}$ consists in passing to the complex conjugate of the wave function (eq. (52)). Let's see how this operator is expressed in the p-representation. Let's develop a generic initial state according to the eigenkets of the linear momentum:

$$|\psi_0\rangle = \int_{\mathbb{R}^3} d^3p \, |\mathbf{p}\rangle \langle \mathbf{p}|\psi_0\rangle$$

It follows

$$\hat{\Theta}|\psi_0\rangle = \int_{\mathbb{R}^3} d^3p \hat{\Theta}\left(\langle \mathbf{p}|\psi_0\rangle |\mathbf{p}\rangle\right) = \int_{\mathbb{R}^3} d^3p \, \langle \mathbf{p}|\psi_0\rangle^* \, \hat{\Theta}|\mathbf{p}\rangle \underset{\text{eq. (29)}}{=} \int_{\mathbb{R}^3} d^3p \, |-\mathbf{p}\rangle \langle \mathbf{p}|\psi_0\rangle^*$$

Performing the change of variable $\mathbf{p} \to -\mathbf{p}$

$$\hat{\Theta}|\psi_0\rangle = \int_{\mathbb{R}^3} d^3p \, |\mathbf{p}\rangle \langle -\mathbf{p}|\psi_0\rangle^*$$

So in the p-representation the wave function changes as $\langle \mathbf{p}|\psi_0\rangle \to \langle -\mathbf{p}|\psi_0\rangle^*$.

3 Time reversal for spin-$1/2$ particle

Let us determine the time-reversed state of an eigenstate of $\hat{\mathbf{S}} \cdot \mathbf{n}$, namely $\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle$ given by the equation (92) which we rewrite here:

$$\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle = \cos\left(\frac{\beta}{2}\right)|+\rangle + e^{i\alpha}\sin\left(\frac{\beta}{2}\right)|-\rangle \tag{55}$$

Nel linguaggio degli spinori:

$$\chi(\mathbf{n}; +) = \cos\left(\frac{\beta}{2}\right)\chi_+ + e^{i\alpha}\sin\left(\frac{\beta}{2}\right)\chi_- \tag{56}$$

In the Appendix (A) we obtained $\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle$ by subjecting $|+\rangle$ to two successive rotations:

$$\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle = \hat{D}_z(\alpha)\,\hat{D}_y(\beta)\,|+\rangle$$

Taking into account the (83), then applying the time reversal operator, we get the time-reversed state:

$$\hat{\Theta}\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle = \hat{\Theta}\left(e^{-\frac{i}{\hbar}\alpha\hat{S}_z}e^{-\frac{i}{\hbar}\beta\hat{S}_z}|+\rangle\right) \tag{57}$$

Angular momentum is odd with respect to time reversal (50):

$$\begin{aligned}
\hat{\Theta}\hat{S}_k\hat{\Theta}^{-1} = -\hat{S}_k \iff \hat{\Theta}\hat{S}_k = -\hat{S}_k\hat{\Theta} \iff \left\{\hat{\Theta}, \hat{S}_k\right\} = 0 \\
\implies \hat{\Theta}e^{-\frac{i}{\hbar}\alpha\hat{S}_k} = -e^{-\frac{i}{\hbar}\alpha\hat{S}_k}\hat{\Theta}, \quad \forall k \in \{x, y, z\} \\
\implies \hat{\Theta}\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle = -\left(e^{-\frac{i}{\hbar}\alpha\hat{S}_z}\underbrace{\hat{\Theta}e^{-\frac{i}{\hbar}\beta\hat{S}_y}}_{=-e^{-\frac{i}{\hbar}\beta\hat{S}_y}\hat{\Theta}}|+\rangle\right)
\end{aligned}$$

i.e.

$$\hat{\Theta}\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle = e^{-\frac{i}{\hbar}\alpha\hat{S}_z}e^{-\frac{i}{\hbar}\beta\hat{S}_y}\hat{\Theta}\,|+\rangle \tag{58}$$

For the aforementioned parity (-1) of the angular momentum:

$$\hat{\Theta}\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle = \eta\left|\hat{\mathbf{S}} \cdot \mathbf{n}; -\right\rangle$$

where η is a phase factor. So

$$e^{-\frac{i}{\hbar}\alpha\hat{S}_z}e^{-\frac{i}{\hbar}\beta\hat{S}_y}\hat{\Theta}\,|+\rangle = \eta\left|\hat{\mathbf{S}} \cdot \mathbf{n}; -\right\rangle \tag{59}$$

Proceeding by rotations:

$$\begin{aligned}
\left|\hat{\mathbf{S}} \cdot \mathbf{n}; -\right\rangle = \hat{D}_z(\alpha)\,\hat{D}_y(\pi+\beta)\,|+\rangle = e^{-\frac{i}{\hbar}\alpha\hat{S}_z}e^{-\frac{i}{\hbar}(\pi+\beta)\hat{S}_y}|+\rangle \\
\implies e^{-\frac{i}{\hbar}\alpha\hat{S}_z}e^{-\frac{i}{\hbar}\beta\hat{S}_y}\hat{\Theta}\,|+\rangle = \eta e^{-\frac{i}{\hbar}\alpha\hat{S}_z}e^{-\frac{i}{\hbar}(\pi+\beta)\hat{S}_y}|+\rangle \\
\underset{\hat{\Theta}=\hat{U}\hat{K}}{\implies} e^{-\frac{i}{\hbar}\alpha\hat{S}_z}e^{-\frac{i}{\hbar}\beta\hat{S}_y}\hat{U}\hat{K}\,|+\rangle = \eta e^{-\frac{i}{\hbar}\alpha\hat{S}_z}e^{-\frac{i}{\hbar}(\pi+\beta)\hat{S}_y}|+\rangle \\
\implies \hat{\Theta}\,|+\rangle = \eta e^{-\frac{i}{\hbar}\pi\hat{S}_y}\hat{K}\,|+\rangle
\end{aligned}$$

i.e.

$$\hat{\Theta} = \eta e^{-\frac{i}{\hbar}\pi\hat{S}_y}\hat{K} \tag{60}$$

Making it explicit $e^{-\frac{i}{\hbar}\pi\hat{S}_y}$

$$\hat{\Theta} = -i\eta\left(\frac{2}{\hbar}\right)\hat{S}_y\hat{K}, \qquad \eta\in\mathbb{C}\mid|\eta|=1 \tag{61}$$

(60) or equivalently (61) is a representation of $\hat{\Theta}$ in the basis $\{|+\rangle, |-\rangle\}$.

Let's now perform time reversal of a generic ket

$$|\psi\rangle = c_+|+\rangle + c_-|-\rangle \tag{62}$$

For this purpose we calculate (vedi A):

$$e^{-\frac{i}{\hbar}\pi\hat{S}_y}|+\rangle = |-\rangle\,, \quad e^{-\frac{i}{\hbar}\pi\hat{S}_y}|-\rangle = -|+\rangle$$

It follows

$$\begin{aligned}\hat{\Theta}|\psi\rangle &= \eta\left(e^{-\frac{i}{\hbar}\pi\hat{S}_y}\hat{K}\right)c_+|+\rangle + \eta\left(e^{-\frac{i}{\hbar}\pi\hat{S}_y}\hat{K}\right)c_-|-\rangle \\ &= \eta c_+^*\underbrace{e^{-\frac{i}{\hbar}\pi\hat{S}_y}|+\rangle}_{=|-\rangle} + \eta c_-^*\underbrace{e^{-\frac{i}{\hbar}\pi\hat{S}_y}|-\rangle}_{=-|+\rangle}\end{aligned}$$

i.e.

$$\hat{\Theta}|\psi\rangle = \eta c_+^*|-\rangle - \eta c_-^*|+\rangle \tag{63}$$

Let's apply again $\hat{\Theta}$

$$\begin{aligned}\hat{\Theta}^2|\psi\rangle &= \hat{U}\hat{K}\left(\eta c_+^*|-\rangle\right) - \hat{U}\hat{K}\left(\eta c_-^*|+\rangle\right) \\ &= \eta e^{-\frac{i}{\hbar}\pi\hat{S}_y}\hat{K}\left(\eta c_+^*|-\rangle\right) - \eta e^{-\frac{i}{\hbar}\pi\hat{S}_y}\hat{K}\left(\eta c_-^*|+\rangle\right) \\ &= -|\eta|^2 c_+ e^{-\frac{i}{\hbar}\pi\hat{S}_y}|-\rangle - |\eta|^2 c_- e^{-\frac{i}{\hbar}\pi\hat{S}_y}|+\rangle \\ &\underset{|\eta|^2=1}{=} -c_+|+\rangle - c_-|-\rangle\end{aligned}$$

i.e.

$$\hat{\Theta}^2|\psi\rangle = -|\psi\rangle\,, \qquad \forall|\psi\rangle\in\mathbb{C}^2$$

So

$$\hat{\Theta}^2 = -\hat{1} \tag{64}$$

Un risultato importante perchè non dipende dalla fase η. Vediamo come si generalizza questo risultato per un generico sistema di spin j. Quindi nella rappresentazione $\{\mathbf{J}^2, J_z\}$

$$\begin{aligned}\hat{\mathbf{J}}^2|jm\rangle &= \hbar^2 j(j+1)|jm\rangle \\ J_z|jm\rangle &= \hbar m|jm\rangle\,, \quad m=-j,...,j\end{aligned} \tag{65}$$

Proposition 4

$$\hat{\Theta}^2|jm\rangle = \begin{cases} -|jm\rangle\,, & j \text{ semi-integer} \\ +|jm\rangle\,, & j \text{ integer}\end{cases} \tag{66}$$

Proof. The system $\{|jm\rangle\}$ is an orthonormal basis in $\mathbb{C}^{2j+1}$:

$$|\psi\rangle = \sum_{m=-j}^{j} |jm\rangle \langle jm|\psi\rangle , \quad \forall |\psi\rangle \in \mathbb{C}^{2j+1}$$

Here $\hat{\Theta} = \eta e^{-\frac{i}{\hbar}\pi \hat{J}_y} \hat{K}$

$$\begin{aligned}
\hat{\Theta} |\psi\rangle &= \eta \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} \hat{K} \left(|jm\rangle \langle jm|\psi\rangle\right) \qquad (67)\\
&= \eta \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} |jm\rangle \langle jm|\psi\rangle^* \\
\hat{\Theta}^2 |\psi\rangle &= \hat{\Theta} \left(\eta \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} |jm\rangle \langle jm|\psi\rangle^* \right) \\
&= \eta e^{-\frac{i}{\hbar}\pi \hat{J}_y} \eta^* \hat{K} |\phi\rangle = e^{-\frac{i}{\hbar}\pi \hat{J}_y} \hat{K} \left(\eta |\phi\rangle\right)
\end{aligned}$$

where

$$\begin{aligned}
|\phi\rangle &\equiv \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} |jm\rangle \langle jm|\psi\rangle^* \\
&\Longrightarrow \hat{K} \left(\eta |\phi\rangle\right) = \eta^* \hat{K} |\phi\rangle \\
&= \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} |jm\rangle \langle jm|\psi\rangle^* \\
&= \eta^* \hat{K} \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} |jm\rangle \langle jm|\psi\rangle^* \\
&= \eta^* \sum_{m=-j}^{j} \underbrace{\hat{K} e^{-\frac{i}{\hbar}\pi \hat{J}_y}}_{=-e^{-\frac{i}{\hbar}\pi \hat{J}_y} \hat{K}} |jm\rangle \langle jm|\psi\rangle^* \\
&= -\eta^* \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} \hat{K} |jm\rangle \langle jm|\psi\rangle^* \\
&= - - \eta^* \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} |jm\rangle \langle jm|\psi\rangle
\end{aligned}$$

Sostituendo in (67):

$$\begin{aligned}
\hat{\Theta}^2 |\psi\rangle &= + |\eta|^2 e^{-\frac{i}{\hbar}\pi \hat{J}_y} \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}\pi \hat{J}_y} |jm\rangle \langle jm|\psi\rangle \\
&= \sum_{m=-j}^{j} e^{-\frac{i}{\hbar}2\pi \hat{J}_y} |jm\rangle \langle jm|\psi\rangle
\end{aligned}$$

$e^{-\frac{i}{\hbar}2\pi \hat{J}_y} |jm\rangle$ rotate $|jm\rangle$ by 2πaround the y-axis:

$$e^{-\frac{i}{\hbar}2\pi \hat{J}_y} |jm\rangle = (-1)^{2j} |jm\rangle$$

So

$$\hat{\Theta}^2 \left|\psi\right\rangle = (-1)^{2j} \left|\psi\right\rangle, \quad \forall \left|\psi\right\rangle \in \mathbb{C}^{2j+1}$$

i.e. the statement. ■

If N is the total number of electrons constituting a quantum system:

$$\begin{aligned}
N &= 1 \Longrightarrow j = \frac{1}{2}, \quad \hat{\Theta}^2 = -\hat{1} \\
N &= 2 \Longrightarrow j = 0, 1, \quad \hat{\Theta}^2 = -\hat{1} \\
N &= 3 \Longrightarrow j \text{ semi-integer}, \quad \hat{\Theta}^2 = -\hat{1}
\end{aligned}$$

i.e.

$$\hat{\Theta}^2 = (-1)^N \hat{1} \tag{68}$$

4 Il Teorema diKramers-Wigner

Consider a time-reversal invariant quantum system, i.e. $\left[\hat{\Theta}, \hat{H}\right] = 0$ where the Hamiltonian includes spin terms. If $|E_n\rangle$ is a generic eigenket of the energy, it follows that $\hat{\Theta}|E_n\rangle$ is an eigenket of the energy with the same eigenvalue. Indeed:

$$\left(\hat{H}\hat{\Theta}\right)|E_n\rangle \underset{\left[\hat{\Theta},\hat{H}\right]=0}{=} \left(\hat{\Theta}\hat{H}\right)|E_n\rangle = \hat{\Theta}\left(\hat{H}|E_n\rangle\right) \underset{E_n\in\mathbb{R}}{=} E_n\left(\hat{\Theta}|E_n\rangle\right)$$

If the spectrum of the Hamiltonian is nondegenerate:

$$\hat{\Theta}|E_n\rangle = e^{i\varphi}|E_n\rangle\,,\ (\varphi\in\mathbb{R}) \Longrightarrow \hat{\Theta}\left(\hat{\Theta}|E_n\rangle\right) = \hat{\Theta}\left(e^{i\varphi}|E_n\rangle\right) = e^{-i\varphi}\hat{\Theta}|E_n\rangle = |E_n\rangle$$

Since $\{|E_n\rangle\}$ is a complete orthonormal system in the appropriate Hilbert space

$$\begin{aligned}\hat{\Theta}^2|E_n\rangle = |E_n\rangle\,,\ \forall E_n\in\sigma\left(\hat{H}\right) &\Longrightarrow \hat{\Theta}^2|\psi\rangle = |\psi\rangle\,,\ \forall|\psi\rangle\in\hat{H}\\ &\Longrightarrow \hat{\Theta}^2 = \hat{1}\end{aligned}$$

But this only occurs for systems of integer spin j. Conversely, for half-integer j is $\hat{\Theta}^2 = -\hat{1}$ so $|E_n\rangle$ and $\hat{\Theta}|E_n\rangle$ are two distinct states with the same energy. In other words, there is degeneracy. Consider, for example, a system consisting of N electrons in an electrostatic field $\mathbf{E}$ of potential $\phi(\mathbf{x})$ (so a single electron has potential energy $V(\mathbf{x}) = -e\phi(\mathbf{x})$). The Hamiltonian is manifestly time-reversal invariant (provided that the electric field is indeed static). By virtue of the previous considerations, the degree of degeneracy of the single electron energy levels is at least $(-1)^N$ i.e. doubly degenerate if N is odd.

This result is interesting for condensed-state physics, where the even or odd number of electrons determines different behaviors. Kramers found this degeneracy by solving the spectrum of the Hamiltonian. Wigner later showed that *Kramers degeneracy* is a consequence of time-reversal invariance. [1]. Possiamo finalmente enunciare:

Theorem 5 *(***Kramers-Wigner Theorem***)*
Hp. *The quantum system is composed of an odd number of fermions, and its Hamiltonian is time-reversal invariant.*
Th. *The spectrum of the Hamiltonian is at least doubly degenerate.*

This theorem is also important for atomic physics: applying an electrostatic field does not definitively remove the degeneracy of the energy levels if the system contains an odd number of electrons. However, the Kramers degeneracy can be removed by applying a magnetic field $\mathbf{B}$ because interaction terms of the type $\mathbf{S}\cdot\mathbf{B}$ appear in the Hamiltonian, which destroy the commutativity between $\hat{\Theta}$ and the Hamiltonian and therefore, the time-reversal invariance.

A 2 Component Spinor Formalism

The spin state space for spin-1/2 particle is the unitary space $\mathbb{C}^2$. The spin observable is represented there by a Hermitian operator $\hat{\mathbf{S}}$ whose Cartesian components according to an inertial frame $(Oxyz)$

are [1]:

$$\hat{S}_x = \frac{\hbar}{2}\left(|+\rangle\langle-| + |-\rangle\langle+|\right) \tag{69}$$
$$\hat{S}_y = \frac{i\hbar}{2}\left(-|+\rangle\langle-| + |-\rangle\langle+|\right)$$
$$\hat{S}_z = \frac{\hbar}{2}\left(|+\rangle\langle+| - |-\rangle\langle-|\right)$$

where $|+\rangle, |-\rangle$ are the autoket of $\hat{S}_z$:

$$\hat{S}_z|\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle \tag{70}$$

Physically, they are the eigenstates of the z-component of the spin. Using a suggestive but effective language, we call $|+\rangle$ *spin up*, and $|-\rangle$ *spin down*. In the operator language, the (69) compose the representations of the operators $\hat{S}_k$ $(k = x, y, z)$ in the basis where $\hat{S}_z$ is diagonal. In fact, assuming the system as an orthonormal basis $\{|+\rangle, |-\rangle\}$:

$$|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv \chi_+ \qquad |-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \chi_-$$

where $\doteq$ means "represented by".

It follows

$$|+\rangle\langle+| \doteq \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$
$$|-\rangle\langle-| \doteq \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$
$$\Longrightarrow \hat{S}_z \doteq \frac{\hbar}{2}\sigma_z \qquad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Any normalized ket:

$$|\psi\rangle = c_+|+\rangle + c_-|-\rangle, \qquad \left(|c_+|^2 + |c_-|^2 = 1\right) \tag{71}$$
$$|\psi\rangle \doteq \begin{pmatrix} c_+ \\ c_- \end{pmatrix} \equiv \chi$$

The column vector χ is called **2-component spinor** . The matrix representations of the other spin components are:

$$\hat{S}_x = \frac{\hbar}{2}\sigma_x \qquad \sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{72}$$
$$\hat{S}_y = \frac{\hbar}{2}\sigma_y \qquad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

The matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{73}$$

are called **Pauli matrices** . These are traceless Hermitian matrices. Furthermore, they satisfy the commutation rules:

$$\{\sigma_k, \sigma_{k'}\} = 2\delta_{kk'}\bar{1}_2 \tag{74}$$
$$[\sigma_k, \sigma_{k'}] = 2i\varepsilon_{kk'r}\sigma_r$$

$\bar{1}_2$is the identity matrix 2×2 . Incidentally, the operators (69) verify the commutation rules:

$$\left\{ \hat{S}_k, \hat{S}_{k'} \right\} = \frac{\hbar^2}{2} \delta_{kk'} \hat{1} \tag{75}$$
$$\left[\hat{S}_k, \hat{S}_{k'} \right] = i\hbar \varepsilon_{kk'r} \hat{S}_r$$

Here $\hat{1}$ is the identity operator in $\mathbb{C}^2$. From (69):

$$\hat{\mathbf{S}}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = \frac{3}{4} \hbar^2 \hat{1} \tag{76}$$
$$\left[\hat{\mathbf{S}}^2, \hat{S}_k \right] = 0, \quad \forall k \in \{x, y, z\}$$

so that $S_k, S_{k' \neq k}$ are incompatible observables, while $\mathbf{S}^2, S_k$ are compatible observables $\forall k \in \{x, y, z\}$.

From the general theory of angular momentum [1] we know that $\hat{S}_k$ is the generator of rotations around the k-th axis. The corresponding unitary operator (rotation operator) is

$$\hat{D}_k (\phi) = e^{-\frac{i}{\hbar} \phi \hat{S}_k} \tag{77}$$

where ϕ is the rotation angle. Applying the rotation operator (77) to the state ket $|\psi\rangle$, takes us to the ket of the rotated system (we are considering *passive rotations*, i.e., instead of rotating the system, we rotate the state ket).

Definition 5 *For all* $\mathbf{a} = (a_x, a_y, a_z)$ *with* $a_k \in \mathbb{C}$, $\forall k \in \{x, y, z\}$*:*

$$\boldsymbol{\sigma} \cdot \mathbf{a} \equiv \sigma_x a_x + \sigma_y a_y + \sigma_z a_z \tag{78}$$

where $\boldsymbol{\sigma}$ *is the "vector" of Pauli matrices:* $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$*.*

We used quotation marks because the components of $\boldsymbol{\sigma}$ are matrices 2×2. From (73):

$$\boldsymbol{\sigma} \cdot \mathbf{a} = \begin{pmatrix} a_z & a_x - i a_y \\ a_x + i a_y & -a_z \end{pmatrix} \tag{79}$$

The following notable identity holds [1]:

$$(\boldsymbol{\sigma} \cdot \mathbf{a}) (\boldsymbol{\sigma} \cdot \mathbf{b}) = (\mathbf{a} \cdot \mathbf{b}) \bar{1}_2 + i \boldsymbol{\sigma} \cdot (\mathbf{a} \wedge \mathbf{b}), \quad \bar{1}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{80}$$

from which

$$(\boldsymbol{\sigma} \cdot \mathbf{a})^2 = \mathbf{a} \cdot \mathbf{a} \bar{1}_2 \tag{81}$$
$$\mathbf{a} \in \mathbb{R}^3 \Longrightarrow (\boldsymbol{\sigma} \cdot \mathbf{a})^2 = |\mathbf{a}|^2 \bar{1}_2, \quad |\mathbf{a}|^2 = \sqrt{a_x^2 + a_y^2 + a_z^2}$$

If $\mathbf{a} = \mathbf{n}$ (unity vector)

$$(\boldsymbol{\sigma} \cdot \mathbf{n})^2 = \bar{1}_2$$
$$(\boldsymbol{\sigma} \cdot \mathbf{n})^3 = (\boldsymbol{\sigma} \cdot \mathbf{n})^2 (\boldsymbol{\sigma} \cdot \mathbf{n}) = \boldsymbol{\sigma} \cdot \mathbf{n}$$
$$(\boldsymbol{\sigma} \cdot \mathbf{n})^4 = (\boldsymbol{\sigma} \cdot \mathbf{n})^2 (\boldsymbol{\sigma} \cdot \mathbf{n})^2 = \bar{1}_2$$
$$\ldots$$

that is

$$(\boldsymbol{\sigma}\cdot\mathbf{n})^k = \begin{cases} \bar{1}_2, & k \text{ pari} \\ \boldsymbol{\sigma}\cdot\mathbf{n}, & k \text{ dispari} \end{cases} \tag{82}$$

Relative to the spin degrees of freedom only, the rotation operator of an angle ϕ around an oriented direction $\mathbf{n}$ is [1]:

$$\hat{D}(\mathbf{n},\phi) = e^{-\frac{i}{\hbar}\phi\hat{\mathbf{S}}\cdot\mathbf{n}} \tag{83}$$

$s = 1/2 \Longrightarrow \hat{\mathbf{S}} \doteq \frac{\hbar}{2}\boldsymbol{\sigma}$

$$\hat{D}(\mathbf{n},\phi) \doteq e^{-i\left(\frac{\phi}{2}\right)\boldsymbol{\sigma}\cdot\mathbf{n}} \tag{84}$$

Let's make the matrix explicit on the second member (2×2):

$$A \equiv -i\left(\frac{\phi}{2}\right)\boldsymbol{\sigma}\cdot\mathbf{n} \Longrightarrow e^A = \sum_{k=0}^{+\infty}\frac{A^k}{k!} = \bar{1}_2 + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \frac{A^4}{4!} + ...$$

$$A^2 = -\left(\frac{\phi}{2}\right)^2(\boldsymbol{\sigma}\cdot\mathbf{n})^2$$

$$A^3 = A^2A^3 = i\left(\frac{\phi}{2}\right)^3(\boldsymbol{\sigma}\cdot\mathbf{n})^3$$

$$A^3 = A^3A = \left(\frac{\phi}{2}\right)^4(\boldsymbol{\sigma}\cdot\mathbf{n})^4$$

It follows

$$e^{-i\left(\frac{\phi}{2}\right)\boldsymbol{\sigma}\cdot\mathbf{n}} = \bar{1}_2\underbrace{\left[1-\frac{1}{2!}\left(\frac{\phi}{2}\right)^2+\frac{1}{4!}\left(\frac{\phi}{2}\right)^4+...\right]}_{=\cos\left(\frac{\phi}{2}\right)} - i(\boldsymbol{\sigma}\cdot\mathbf{n})\underbrace{\left[\frac{\phi}{2}-\frac{1}{3!}\left(\frac{\phi}{2}\right)^3+...\right]}_{=\sin\left(\frac{\phi}{2}\right)}$$

That is

$$e^{-i\left(\frac{\phi}{2}\right)\boldsymbol{\sigma}\cdot\mathbf{n}} = \bar{1}_2\cos\left(\frac{\phi}{2}\right) - i(\boldsymbol{\sigma}\cdot\mathbf{n})\sin\left(\frac{\phi}{2}\right) \tag{85}$$

we finally obtain the matrix representation of the operator (84) in the representation where $\hat{S}_z$ is diagonal.

$$\hat{D}(\mathbf{n},\phi) \doteq e^{-i\left(\frac{\phi}{2}\right)\boldsymbol{\sigma}\cdot\mathbf{n}} = \begin{pmatrix} \cos\left(\frac{\phi}{2}\right) - in_z\sin\left(\frac{\phi}{2}\right) & (-in_x - n_y)\sin\left(\frac{\phi}{2}\right) \\ (n_y - in_x)\sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right) + in_z\sin\left(\frac{\phi}{2}\right) \end{pmatrix} \tag{86}$$

The unitary operator (86) rotates the state kets of any spin 1/2 system:

$$|\psi\rangle = c_+|+\rangle + c_-|-\rangle, \qquad |c_+|^2 + |c_-|^2 = 1 \tag{87}$$

$$|\psi\rangle \longrightarrow |\psi\rangle_R = e^{-\frac{i}{\hbar}\phi\hat{\mathbf{S}}\cdot\mathbf{n}}|\psi\rangle$$

In the language of spinors:

$$|\psi\rangle \doteq \chi = c_+\chi_+ + c_-\chi_- = \begin{pmatrix} c_+ \\ c_- \end{pmatrix} \tag{88}$$

$$\chi \longrightarrow \chi_R = e^{-i\left(\frac{\phi}{2}\right)\boldsymbol{\sigma}\cdot\mathbf{n}}\chi$$

Let's determine the eigenspinor of $\boldsymbol{\sigma} \cdot \mathbf{n}$ with eigenvalue $+1$, where $\mathbf{n}$ is an arbitrarily assigned unit vector defined by the polar angle β and the azimuthal angle α. Instead of solving the eigenvalue equation $(\boldsymbol{\sigma} \cdot \mathbf{n})\,\chi = \chi$, we use the rotation operator (86) Specifically, the eigenspinor we are looking for is the result of two successive rotations of the spinor $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, the first by an angle β around the y-axis in a counterclockwise direction, the second by an angle a around the z-axis in a counterclockwise direction. The result of the first rotation is the spinor:

$$e^{-i\left(\frac{\beta}{2}\right)\sigma_y}\chi_+ = \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) & -\sin\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right) & \cos\left(\frac{\beta}{2}\right) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right) \end{pmatrix} \tag{89}$$

By rotating the spinor (89) around the z-axis by an angle α, we obtain the eigenspinor we are looking for:

$$\chi = e^{-i\left(\frac{\alpha}{2}\right)\sigma_z} \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha}{2}} & 0 \\ 0 & e^{i\frac{\alpha}{2}} \end{pmatrix} \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha}{2}}\cos\left(\frac{\beta}{2}\right) \\ e^{i\frac{\alpha}{2}}\sin\left(\frac{\beta}{2}\right) \end{pmatrix} \tag{90}$$

Let's check:

$$(\boldsymbol{\sigma} \cdot \mathbf{n}) \begin{pmatrix} e^{-i\frac{\alpha}{2}}\cos\left(\frac{\beta}{2}\right) \\ e^{i\frac{\alpha}{2}}\sin\left(\frac{\beta}{2}\right) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\alpha}{2}}\cos\left(\frac{\beta}{2}\right) \\ e^{i\frac{\alpha}{2}}\sin\left(\frac{\beta}{2}\right) \end{pmatrix}$$

The eigenspinor (90) is the eigenket representation of $\hat{\mathbf{S}} \cdot \mathbf{n}$ with eigenvaluecon $+\hbar/2$:

$$\left(\hat{\mathbf{S}} \cdot \mathbf{n}\right) \left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle = \frac{\hbar}{2} \left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle \tag{91}$$

More specifically

$$\begin{aligned} \left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle &\doteq \frac{\hbar}{2} \begin{pmatrix} e^{-i\frac{\alpha}{2}}\cos\left(\frac{\beta}{2}\right) \\ e^{i\frac{\alpha}{2}}\sin\left(\frac{\beta}{2}\right) \end{pmatrix} \\ \left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle &= e^{-i\frac{\alpha}{2}}\cos\left(\frac{\beta}{2}\right)|+\rangle + e^{i\frac{\alpha}{2}}\sin\left(\frac{\beta}{2}\right)|-\rangle \\ &= e^{-i\frac{\alpha}{2}}\left[\cos\left(\frac{\beta}{2}\right)|+\rangle + e^{i\alpha}\sin\left(\frac{\beta}{2}\right)|-\rangle\right] \end{aligned}$$

Except for an inessential phase factor:

$$\left|\hat{\mathbf{S}} \cdot \mathbf{n}; +\right\rangle = \cos\left(\frac{\beta}{2}\right)|+\rangle + e^{i\alpha}\sin\left(\frac{\beta}{2}\right)|-\rangle \tag{92}$$

A.1 SO(3) and SU(2)

A rotation in $\mathbb{R}^3$ is an orthogonal transformation. Specifically, it is realized by a unimodular orthogonal matrix R ($\det R = +1$) belonging to the group SO(3). The latter is a subgroup of O(3) whose elements are the orthogonal matrices, therefore with $\det = \pm 1$. We then established that to a rotation in physical space, we can associate a unitary transformation in the unitary space $\mathbb{C}^2$ of spin states for a spin 1/2 system.

A straightforward calculation shows that the unitary matrix (86) is unimodular. The more general unimodular unitary matrix 2×2 is

$$U(a,b) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \tag{93}$$

whose matrix elements $a, b \in \mathbb{C}$ satisfy the unimodularity condition:

$$|a|^2 + |b|^2 = 1 \tag{94}$$

so $|b| = \sqrt{1 - |a|^2}$. Writing $a = |a| e^{i\alpha}$, $b = |b| e^{i\beta}$:

$$U(\alpha, \beta, a) = \begin{pmatrix} |a| e^{i\alpha} & \sqrt{1 - |a|^2} e^{i\beta} \\ -\sqrt{1 - |a|^2} e^{-i\beta} & |a| e^{-i\alpha} \end{pmatrix}, \quad \forall \alpha, \beta \in \mathbb{R}, \ \forall |a| \in (0, 1] \tag{95}$$

Conclusion 3 *A 2×2 unimodular unitary matrix is defined up to three real parameters.*

Definition 6 *In (93) The coefficients a, b are called* **Cayley–Klein parameters**. *They were already known in the kinematics of rigid bodies, in particular gyroscopes.*

Recall that for any unitary matrix U is $|\det U| = 1$ so $\det U$ is a phase factor:

$$\det U = e^{i\gamma}, \quad \gamma \in \mathbb{R} \tag{96}$$

It follows that the most general unitary matrix 2×2 is

$$U = \begin{pmatrix} a & b \\ -b^* e^{i\gamma} & a^* e^{i\gamma} \end{pmatrix}, \quad \forall \gamma \in \mathbb{R}, \quad |a|^2 + |b|^2 = 1 \tag{97}$$

With respect to the row-by-column product operation, the set of unitary matrices assumes the algebraic structure of a non-Abelian group and is denoted by U(2). The unimodular set of unitary matrices is a subset of U(2) from which it inherits the group properties, so it is a subgroup of U(2) and is denoted by SU(2) (where S stands for special).

The matrix (86) is therefore an element of SU(2).

A.1.1 Parameterization of SU(2)

Eq. (93) with the unimodularity condition (94) constitutes a parametrization of SU(2); on the other hand, (86) is also the most general unitary matrix whose free parameters are $\phi, \mathbf{n}$. We thus have two distinct parametrizations:

$$U(a, b) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \tag{98}$$

$$U(\phi, \mathbf{n}) = \bar{1}_2 \cos\left(\frac{\phi}{2}\right) - i(\boldsymbol{\sigma} \cdot \mathbf{n}) \sin\left(\frac{\phi}{2}\right)$$

The transformation equations $(\phi, \mathbf{n}) \to (a, b)$:

$$a(\phi, \mathbf{n}) = \cos\left(\frac{\phi}{2}\right) - in_z \sin\left(\frac{\phi}{2}\right), \quad b(\phi, \mathbf{n}) = (-in_x - n_y) \sin\left(\frac{\phi}{2}\right) \tag{99}$$

From the above, there is a correspondence between orthogonal transformations in $\mathbb{R}^3$ and unimodular transformations in $\mathbb{C}^2$. Specifically, there is a linear map:

$$\Lambda : \mathrm{SU}(2) \longrightarrow \mathrm{SO}(3)$$

It can be shown [3] that Λ is a non-injective map, so it is not an isomorphism. Precisely, the unimodular transformations $U(\phi, \mathbf{n})$ e $-U(\phi, \mathbf{n})$ correspond to the same orthogonal transformation in SO(3).

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