For Roger Penrose the “negative frequencies” in Quantum Mechanics are “bad news”

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Abstract

In relativistic quantum mechanics, free particle states with negative energy (negative frequency of the wave function) are not easy to interpret.

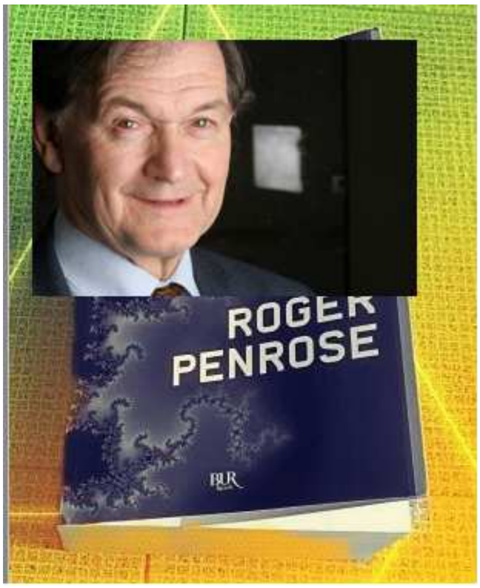

Figure 1: Nobel Prize winner Sir Roger Penrose.

1 Classical mechanics (non-relativistic and relativistic)

In the motion of a particle not subjected to external force fields (*free particle*), the appearance of negative energy states is a consequence of the theory of special relativity formulated by Albert Einstein at the beginning of the last century. On the other hand, in the non-relativistic limit (low speeds compared to the speed c of light in vacuum) there are no states of negative energy. In fact, in this case the total mechanical energy (i.e. kinetic+potential) is reduced to just the kinetic term $(1/2)\,mv^2$ which is never negative. In the case of relativistic motion, however, the energy of a free particle of mass m is such that [1]

$$E^2 = m^2c^4 + c^2\,|\mathbf{p}|^2 \tag{1}$$

where $\mathbf{p}$ is the impulse (i.e. momentum). From (1)

$$E = \pm\sqrt{m^2c^4 + c^2\,|\mathbf{p}|^2} \tag{2}$$

hence the ambiguity of the sign and therefore the appearance of states with negative energy. Figure 2 illustrates the two cases (non-relativistic and relativistic).

In the first case only states are possible $E \geq 0$, so $E = 0$ is the minimum possible value (state of rest in the corresponding inertial reference system). In the second case both the states $E \geq mc^2$ and the states $E \leq -mc^2$ are possible. We then see that for $E > 0$, the value $+mc^2$ defines the state of rest (*rest energy*). However, states with $E < 0$ are not observable. In fact, given the

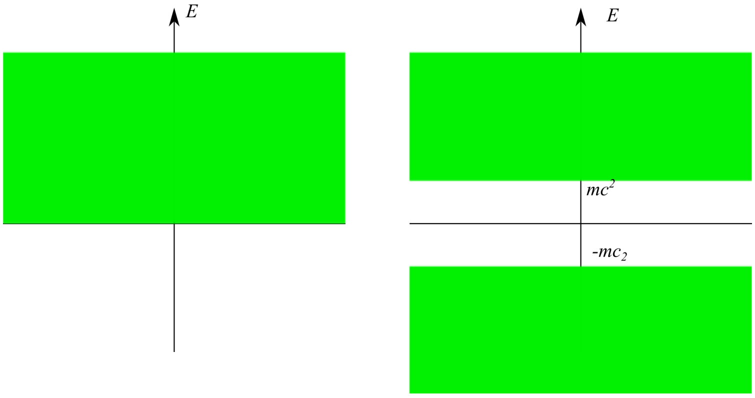

Figure 2: The first graph refers to the non-relativistic motion of a free particle. The second graph refers to the corresponding relativistic motion.

initial mechanical state defined by a value $|\mathbf{p}_0|$ of the impulse module to which the initial energy corresponds:

$$E_0 = +\sqrt{m^2c^4 + c^2 |\mathbf{p}_0|^2} > mc^2, \tag{3}$$

it turns out that this value is conserved during the motion since we are considering a free particle which is a particular case of a conservative system. Put another way, states with $E < 0$ are automatically excluded from the appropriate initial conditions.

2 The quantum particle with zero spin

The quantum case is very different. More specifically, in the non-relativistic regime the dynamic evolution of the quantum state of a system consisting of a single particle is controlled by the Schrödinger equation if the spin is zero, otherwise by the Pauli equation [2]. In relativistic motion, in the case $s = 0$ (s is the spin quantum number), Klein, Gordon and Fok (and perhaps Schrödinger himself before writing his famous equation) in 1926 derived a quantum-relativistic equation:

$$\boldsymbol{\nabla}^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \frac{1}{\lambda_c^2}\psi = 0 \tag{4}$$

known as the *Klein-Gordon equation*. Here $\lambda_c > 0$ is a characteristic length known as the *Compton wavelength* of the particle:

$$\lambda_c = \frac{\hbar}{mc} \tag{5}$$

Note that in the case of photons is $\lambda_c = +\infty$ since $m = 0$, and the (4) reduces to the D'Alembert equation. This result is not surprising because the equation describes the propagation of an electromagnetic wave. To solve the (4) the standard procedure in quantum mechanics is applied, i.e. the search for solutions of the monochromatic plane wave type which, as is well known, describe states in which the observables impulse and energy have values uniquely determined. Once the calculations have been performed, negative energy states appear which, unlike the non-quantum case, cannot be ignored, because they make up the eigenvalue spectrum of a Hermitian operator. More specifically, an eigenvalue $E < 0$ corresponds to the energy eigenfunction:

$$\psi(\mathbf{x}, t) = A \exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x} + |E|\, t)\right] \tag{6}$$

Remembering the relationships between energy and frequency ω, and between impulse and wave vector $\mathbf{k}$

$$\psi\left(\mathbf{x},t\right)=A\exp\left[i\left(\mathbf{k}\cdot\mathbf{x}+\left|\omega\right|t\right)\right] \tag{7}$$

so the frequency appears with the "wrong sign", i.e. $\omega<0$ instead of $\omega>0$. In [3], the Nobel Prize winner Sir Roger Penrose, jokingly referring to this circumstance by classifying it as "bad news", proposes an ingenious argument based on the extension of the Fourier series to the complex field and in particular , to the theory of holomorphic functions.

Mathematically, the appearance of negative energy states is a consequence of the order of the differential equation (4). In fact, this equation is of the second order with respect to the time derivative. On the other hand, the Schrödinger equation being of the first order with respect to the time derivative, does not give rise to states with negative energy. Furthermore, increasing the order changes the corresponding Cauchy problem regarding the initial conditions. This destroys the possibility of interpreting $\left|\psi\right|^2$ as the probability density of finding the particle in a given point for a given instant (Born statistical interpretation), since particular initial conditions return $\left|\psi\right|^2<0$ which is an evident nonsense (a probability cannot be negative!). In this framework, the only possible interpretation is the following: $\left|\psi\right|^2=$ electric charge density. Therefore the Klein-Gordon (K-G) equation should describe spin-zero but electrically charged particles. But this interpretation also appears cumbersome: through a sophisticated mathematical device [4], is discovered that a given solution of the K-G uniquely corresponds to a second solution which describes the motion of a new particle having the same mass as the assigned particle, but opposite electric charge. It is the so-called *antiparticle*. In the cited article, the quantum-relativistic motion of the π^- meson is studied which, as is well known, has $s=0$ and electric charge $q=-e$, where e is the absolute value of the charge of the electron. It follows that its antiparticle is the π^+ meson.

3 Solutions of the D'Alembert Equation

The D'Alembert equation also has similar problems. In 1940 the Italian mathematician Luigi Fantappiè elaborated [6] a suggestive interpretation of the waves with negative frequency (as well as for the D'Alembert equation also for the K-G and for the Dirac equation (spin particles 1/2)), asserting that these are waves coming from the "future" and propagating towards the "past". In a quantum context this has shocking implications since the antiparticle would appear as the same particle moving backwards in time.

4 Conclusions

This brief review of the interpretative problems of relativistic quantum mechanics seems foreign to semiconductor physics. However, the attentive reader has certainly noticed from Figure 2 that in the relativistic case, the $2mc^2$ energy interval appears as a gap or rather, as a potential barrier. Incidentally, in 1937 Oscar Klein demonstrated that under appropriate conditions, an electron can penetrate this barrier via a tunneling process, passing from an $E>0$ state to an $E<0$ state. This process (known as *Klein's paradox*) has recently been observed in graphene.

References

[1] Landau L.D., Lifsits E.M., Fisica Teorica 2. Teoria dei campi. Editori Riuniti

[2] Caldirola P., Prosperi G., Cirelli R. Introduzione alla fisica teorica. UTET

[3] Penrose R. The Road to Reality: A Complete Guide to the Laws of the Universe.

[4] Colozzo M. The Klein-Gordon Equation .

[5] Colozzo M. The Problem of the "Negative Frequencies" of the Solutions of the D'Alembert Equation.

[6] Arcidiacono G., Fantappié e gli universi. Nuove vie della scienza.

[7] Fasano A., Marmi S., Analytical Mechanics.