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Only in the standard representation the Dirac theory is a quantum theory of a single fermion

Abstract It is shown that the relativistic quantum mechanics of a single fermion can be developed only on the basis of the standard representation of the Dirac bispinor. As in the nonrelativistic quantum mechanics, the arbitrariness in defining the bispinor, as a four-component wave function, is restricted by its multiplication by an arbitrary phase factor. We reveal the role of the large and small components of the bispinor, establish their link in the nonrelativistic limit with the Pauli spinor, as well as explain the role of states with negative energies. The Klein tunneling is treated here as a physical phenomenon analogous to the propagation of the electromagnetic wave in a medium with negative dielectric permittivity and permeability. For the case of localized stationary states we define the effective one-particle operators which act in the space of the large component but contain the contributions of both components. The effective operator of energy is presented in a compact analytical form.

Keywords Dirac equation · Klein tunneling · intrinsic parity · spin-orbit interaction

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1 Introduction

This work is a further development of our one-particle formulation [1] of the Dirac theory. In part, this is motivated by the criticism of our solution of the Klein paradox in another "one-particle" approach [2], developed on the basis of the Foldy-Wouthuysen (FW) representation. The point is that our solution implies the existence of the Klein tunneling, while the approach [2] is not. Moreover, another approach to the Klein paradox, developed within the framework of quantum field theory (see [3]), also denies the Klein tunneling. In this connection, we can not but respond to this criticism.

However, it is perhaps more important to defend the basic idea of our approach, that Dirac’s theory can really be represented as an internally consistent quantum theory of an individual particle with half-integer spin. We must overcome the prevailing view that the Dirac theory can not be constructed as a single-particle theory. Among the existing ones, even the approach [2], presented by its author as “single-particle”, is rather a two-particle (electron-positron) approach. In this connection our task is twofold. On the one hand we have to put forward arguments against those existing results which make it impossible a one-particle formulation of the Dirac theory, and on the other hand we have to present more sound arguments in favour of our approach [1].

We begin our analysis with the well-known fact that the Dirac equation is not unique, because the Dirac matrices and, consequently, the Dirac bispinor are determined up to unitary transformations. In the standard approach, the choice of a representation of the Dirac bispinor is only a matter of convenience, since all representations are equivalent from the group-theoretical point of view. At the
same time, if we want to develop a relativistic generalization of the Pauli theory, we must take into account that the "nonrelativistic wave function" is determined to within a phase factor; more wide arbitrariness is unacceptable.

As is known, any unitary representation of the Dirac's bispinor is also determined up to a phase factor. Thus, in developing the Dirac theory as relativistic quantum mechanics of a single fermion we must be guided by the following three considerations:

(a) there is only one unitary representation of the Dirac bispinor in which the Dirac theory admits a one-particle quantum-mechanical formulation;
(b) this representation must obey the requirement of the 'nonrelativistic calibration of the relativistic quantum probability' – in this representation the Dirac bispinor, as a four-component probability amplitude, must be compatible in the nonrelativistic limit with the Pauli spinor;
(c) the nonrelativistic wave function is determined to within a phase factor; more wide arbitrariness is unacceptable.

As will be shown, only the standard representation corresponds to this calibration.

2 Equations for the large and small components of the Dirac bispinor

In the standard representation the Dirac equation with the scalar electric potential \( e\Phi(r) \) and vector potential \( eA(r) \) has the form

\[
\frac{i\hbar}{\partial t} \Psi = H_D \Psi; \quad H_D = \alpha (\hat{p} + eA) + e\phi + \beta mc^2, \tag{1}
\]

where \( \alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \), \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \); here \( \sigma_x, \sigma_y \) and \( \sigma_z \) are the Pauli matrices;

\( \Phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} \) and \( \chi = \begin{pmatrix} \chi^+ \\ \chi^- \end{pmatrix} \) are the "large" (upper) and "small" (lower) components of the bispinor \( \Psi = \begin{pmatrix} \Phi \\ \chi \end{pmatrix} \), respectively; \( e \) is the electrical charge of the Dirac particle, \( m \) is its mass; \( \hat{p} = -i\hbar \nabla; \) \( r \) is the spatial variable. The corresponding continuity equation is

\[
\frac{\partial W}{\partial t} + \nabla J = 0; \quad W = \Phi^\dagger \phi + \chi^\dagger \chi, \quad J = e(\Phi^\dagger \sigma \chi + \chi^\dagger \sigma \phi). \tag{2}
\]

In order to reveal the key role of the standard representation, we have first to study in this representation the main properties of the stationary Dirac equation. For this purpose let us remind (see \[1\]) that the large and small components of the Dirac bispinor for the particle with the energy \( E \), when

\[
\Phi(r,t) = \Phi(r; E)e^{-iEt/\hbar}, \quad \chi(r,t) = \chi(r; E)e^{-iEt/\hbar}, \tag{3}
\]

allow one to introduce the notion of the "heavy" and "light" quasiparticles, whose dynamics is Schrödinger-like for any (positive) energy \( E \). Indeed, Eq. (1) can be written in the form

\[
c\sigma \hat{\pi} \chi + (e\phi - E + mc^2) \Phi = 0, \quad c\sigma \hat{\pi} \phi + (e\phi - E - mc^2) \chi = 0; \tag{4}
\]

\( \hat{\pi} = \hat{p} - \frac{e}{c} A \). As was shown in \[1\], the first equation in (4) can be written as a generalized Pauli equation for \( \Phi \), and the second one can be written as an equation that links the spinors \( \chi \) and \( \phi \):

\[
\hat{H}_M \Phi = c\phi, \quad \chi = \frac{\sigma \hat{\pi} \phi}{2Mc}; \quad M = m + \frac{e - e\phi}{2c^2}, \quad \epsilon = E - mc^2; \tag{5a}
\]

\[
\hat{H}_M = \sigma \frac{\hat{\pi}}{2M} \sigma + c\phi = \frac{\hat{\pi}^2}{2M} - \frac{i\hbar}{2} \left( \sigma \nabla \left( \frac{1}{M} \right) \sigma \hat{\pi} + c\phi - \frac{e\hbar}{2Mc} \sigma \mathbf{H}; \quad \mathbf{H} = [\nabla \times \mathbf{A}]; \tag{5b}
\]

\[
W = \Phi^\dagger \phi + \frac{1}{4c^2} \left( \frac{\sigma \hat{\pi} \phi}{M} \right) \left( \frac{\sigma \hat{\pi} \phi}{M} \right)^\dagger; \quad J = \frac{1}{2} \left[ \phi^\dagger \sigma \left( \frac{\sigma \hat{\pi} \phi}{M} \right) + \left( \frac{\sigma \hat{\pi} \phi}{M} \right)^\dagger \sigma \phi \right]. \tag{5c}
\]
In (5a), the generalized Pauli equation with the Hermitian operator $\hat{H}_M$ describes a quasiparticle moving in the usual three-dimensional space with the energy $\epsilon$ (measured from the level that corresponds to the rest energy $+mc^2$ of this quasiparticle) and effective mass $M$ that carries information about the Lorentzian symmetry of the four-dimensional space-time (in solid state theory, this quasiparticle is an analog of the Bloch electron at the bottom of the conduction band). The continuity of the probability density $W$ in (2), the probability current density $J$ and the spinor $\chi$ at the points of discontinuity of $\phi(r)$ and $\bar{A}(r)$ is provided by the continuity of the spinors $\Phi$ and $\frac{1}{\mu}\sigma\pi\hat{\phi}$.

The system of Eqs. (10a) can also be written in another equivalent form: the second equation in (4) can be written as a generalized Pauli equation for the spinor $\chi$, and the second one can be written as an equation that links the spinor $\Phi$ with the spinor $\chi$:

$$\frac{d}{dt}\chi = \epsilon\chi, \quad \Phi = \frac{\sigma\pi\chi}{2\mu c}; \quad \mu = -m + \frac{\epsilon - e\phi}{2e^2}, \quad \epsilon = \epsilon + 2mc^2; \quad (6a)$$

$$\hat{H}_\mu \chi = \epsilon'\chi, \quad \Phi = \frac{\sigma\pi\chi}{2\mu c}; \quad \mu = -m + \frac{\epsilon - e\phi}{2e^2}, \quad \epsilon' = \epsilon + 2mc^2; \quad (6b)$$

$$W = \chi^\dagger \chi + \frac{1}{4e^2} \left( \frac{\sigma\pi\chi}{\mu} \right) \left( \frac{\sigma\pi\chi}{\mu} \right)^\dagger; \quad J = \frac{1}{2} \left[ \chi^\dagger \sigma \left( \frac{\sigma\pi\chi}{\mu} \right) + \left( \frac{\sigma\pi\chi}{\mu} \right)^\dagger \sigma \chi \right]. \quad (6c)$$

The generalized Pauli equation in (6a) describes a quasiparticle moving in the usual three-dimensional space with the energy $\epsilon'$ (measured from the level that corresponds to the rest energy $-mc^2$ of this quasiparticle) and effective mass $\mu$ that carries information about the Lorentzian symmetry of the four-dimensional space-time (this quasiparticle is an analog of the Bloch electron at the top of the valence band); since $M - \mu = m > 0$, quasiparticles with the effective masses $M$ and $\mu$ will be further named "heavy" and "light", respectively. The continuity of the probability density $W$, the probability current density $J$ and the spinor $\phi$ is now provided by the continuity of the spinors $\chi$ and $\frac{1}{\mu}\sigma\pi\chi$.

At first glance, due to the different effective masses in Eqs. (5a) and (6a), the quantum dynamics of the heavy and light quasiparticles differ cardinaly from each other even in the free case. But this is not so. To show this, let us rewrite Eqs. (5a) and (6a) in the form which is more convenient for their comparison. For this purpose we have to multiply Eq. (5a) by $2M$ and then combine together the terms $e\phi\Phi$ and $e\Phi$. Besides, let $\pi = -ih\bar{D}$, where $\bar{D} = \nabla - \frac{e}{\mu}\bar{A}$. As a result, we obtain

$$\left\{ \frac{D^2}{2M} - \left( \nabla \ln |\bar{M}| \right) \bar{D} - i\sigma \left[ \left( \nabla \ln |\bar{M}| \right) \times \bar{D} \right] + \frac{e}{\hbar c} \sigma H + k_0^2 \bar{M} \bar{\mu} \right\} \Phi = 0; \quad (7)$$

Similarly, Eq. (6a) for $\chi$ is equivalent to

$$\left\{ \frac{D^2}{2M} - \left( \nabla \ln |\bar{\mu}| \right) \bar{D} - i\sigma \left[ \left( \nabla \ln |\bar{\mu}| \right) \times \bar{D} \right] + \frac{e}{\hbar c} \sigma H + k_0^2 \bar{\mu} \bar{\mu} \right\} \chi = 0 \quad (8)$$

Taking into account that

$$\nabla \ln |\bar{M}| = \frac{e}{2M M_0 c^2} E, \quad \nabla \ln |\bar{\mu}| = \frac{e}{2\mu_0 c^2} E, \quad E = -\nabla \phi,$$

we arrive at the conclusion that Eqs. (7) and (8) coincide with each other for the arbitrary vector function $\bar{A}(r)$ and constant scalar potential $\phi$ (that is, $E = 0$).

For a free particle these spinors obey the Klein-Gordon equations $(-c^2\hbar^2 \Delta + m^2 c^4)\Phi, \chi = E^2\Phi, \chi$. And, for the following, it is important to note that only one of these (coinciding by form) equations is relevant. Namely, for a free particle the Dirac equations (4) are equivalent either the system of equations (10a) or the system of equations (10b):

$$(-c^2\hbar^2 \Delta + m^2 c^4)\Phi = E^2\Phi, \quad \chi = \frac{\sigma\pi\phi}{2M_0 c}; \quad (10a)$$

$$(-c^2\hbar^2 \Delta + m^2 c^4)\chi = E^2\chi, \quad \Phi = \frac{\sigma\pi\chi}{2\mu_0 c}. \quad (10b)$$
As a system of two ordinary differential equations of the second order for the functions \( \psi \) here corresponding Pauli equation in independent solutions. As such a solution, we can take a spinor proportional to the function

\[
\chi \approx -\frac{i\hbar}{2mc} \sigma \nabla \phi.
\]

Note that the generalized Pauli equation (6a) exhibits similar properties in the limit \( \epsilon' \rightarrow 0 \). In this case it reduces to the Pauli equation for a particle with the mass \( -m \):

\[
\frac{\hbar^2}{2m} \nabla^2 \chi \approx \epsilon' \chi, \quad W \approx \phi \phi^\dagger, \quad \mathbf{J} \approx -\frac{i\hbar}{2m} \left( \nabla \phi \phi^\dagger - \phi \nabla \phi^\dagger \right); \quad \chi \approx -\frac{i\hbar}{2mc} \sigma \nabla \phi.
\]

As is seen, for \( \epsilon = 0 \) the small component is zero, and for \( \epsilon' = 0 \) the large component is zero. For this reason, in the standard approach, only the large component \( \phi \) is associated with the upper continuum of states of the Dirac particle, while the small component \( \chi \) is associated with the lower continuum of its states (or, eventually, with the upper continuum of states of the Dirac antiparticle). As a consequence, the FW representation, where these two components are separated from each other, seems to obey the nonrelativistic calibration.

But this is not the case. Indeed, as it follows from (11), for however small (but nonzero) values of \( \epsilon \) the small component is not less essential than the large component, because the probability current density is nonzero together with \( \chi \); \( |\mathbf{J}| \sim |\chi| \sim |\nabla \phi| \). Thus, at this stage of our analysis only the standard representation reproduces the Pauli dynamics. Nevertheless, there is necessity in a more careful analysis of the compatibility of the Dirac bispinor in the standard representation with the Pauli spinor in the nonrelativistic limit. For this purpose we have to anew analyse a complete system of independent solutions of the stationary Dirac equation for a free Dirac particle whose momentum is collinear to the \( OZ \)-axis. In particular, by the example of this simplest problem we have to show that the part of independent solutions in this problem – the (odd) eigenstates of the parity operator – disappears when \( \epsilon = 0 \) but is essential for however small (but nonzero) values of \( \epsilon \).

3 A complete sets of independent solutions for a free particle moving in \( z \)-direction

When the particle momentum is strictly collinear to the \( OZ \) axis, we actually deal with a particle with a single external (translational) degree of freedom. In this case, the system of Eqs. (1) splits into two independent subsystems equations for the components of the spinors \( \Phi \) and \( \chi \) which depend on the positive parameter \( E \) and the only spatial variable \( z \):

\[
-ic \frac{d\chi}{dz} + mc^2 \phi = E\phi, \quad -ic \frac{d\phi}{dz} - mc^2 \chi = E\chi; \tag{13}
\]

\[
-ic \frac{d\chi}{dz} + mc^2 \phi = E\phi, \quad ic \frac{d\phi}{dz} - mc^2 \chi = E\chi. \tag{14}
\]

In line with Section 2 these equations can be rewritten in the form

\[
\hat{H}_M \begin{pmatrix} \phi \cr \phi \end{pmatrix} = \epsilon(E) \begin{pmatrix} \phi \cr \phi \end{pmatrix}, \quad \begin{pmatrix} \chi \cr \chi \end{pmatrix} = -\frac{i\hbar}{2Me} \sigma \frac{d}{dz} \begin{pmatrix} \phi \cr \phi \end{pmatrix}; \quad \hat{H}_M = -\frac{\hbar^2}{2M} \frac{d^2}{dz^2}. \tag{15}
\]

This form is more convenient for comparing these equations, in the nonrelativistic limit, with the corresponding Pauli equation

\[
\hat{H}_m \begin{pmatrix} \psi \cr \psi \end{pmatrix} = \epsilon(E) \begin{pmatrix} \psi \cr \psi \end{pmatrix}; \tag{16}
\]

here \( \psi(z) \) and \( \psi(z) \) are the upper and lower components of the Pauli spinor; the Hamiltonian \( \hat{H}_m \) can be obtained from \( \hat{H}_M \) (see (15)) by substituting the original mass \( m \) for the effective mass \( M \). As a system of two ordinary differential equations of the second order for the functions \( \psi(z) \) and \( \psi(z) \) that describe the subensembles of particles with the spin up and down, this equation has four independent solutions. As such a solution, we can take a spinor proportional to the function \( e^{ipz} \),
where $p_z$ is a constant. After substituting such a spinor to Eqs. (10) we obtain a uniform system of algebraic equations which is solvable when $\epsilon(E) = p_z^2/2m$.

It is important to emphasize that in the nonrelativistic quantum mechanics this equation, connecting the energy of an electron with its momentum, is considered as an equation for the latter, and not vice versa. Thus, we have $p_z = \pm p$, where $p = \sqrt{2mc(E)}$. As a result, we obtain four independent solutions to be eigenvectors of the $z$-projection of the momentum operator $\hat{p}$ (which commutes with $H_m$ in this problem):

$$
\psi_{\pm p}^\pm(z) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{\pm ipz/\hbar}; \quad \psi_{\pm p}^\pm(z) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{\pm ipz/\hbar}.
$$

Another system of independent solutions of Eqs. (10) is presented by the eigenfunctions of the (orbital) parity operator $\hat{P}$ which also commutes with $H_m$ (but does not commute with the momentum operator); $\hat{P}\psi(r, t) = \pm \psi(-r, t)$:

$$
\psi_{\uparrow}^+(r) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cos \left(\frac{p_z}{\hbar} \right); \quad \psi_{\downarrow}^-(r) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \sin \left(\frac{p_z}{\hbar} \right); \quad \psi_{\downarrow}^+(r) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cos \left(\frac{p_z}{\hbar} \right); \quad \psi_{\uparrow}^-(r) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \sin \left(\frac{p_z}{\hbar} \right).
$$

For the following it is important to stress that the case $p = 0$ (i.e., when $E = mc^2$) is exceptional for this problem because two independent solutions – the odd solutions $\psi_{\uparrow}^-(r)$ and $\psi_{\uparrow}^+(r)$ – disappear in this limiting case (though they are essential for a however small value of $p$).

In the Dirac theory, as in the Pauli one, we will take as a searched-for solution a bispinor proportional to $e^{ipz}$. But now, after substituting it into Eqs. (13) and (14) (or Eqs. (15)), we obtain a homogeneous system of algebraic equations, which is solvable when $E^2 = c^2p_z^2 + mc^4$. Following the nonrelativistic theory, we will consider this equality as an equation for the parameter $p_z$. Now $p_z = \pm p$, where $p = \sqrt{E^2 - mc^2 / c^2} \equiv \sqrt{2\gamma(E)M(E)} \geq 0$. As a result, for a given (positive) $E$ we have four solutions

$$
\psi_{+p, \uparrow}^E(z) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{\pm p}{2Mc} e^{\pm ipz/\hbar}; \quad \psi_{+p, \downarrow}^E(z) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \frac{\pm p}{2Mc} e^{\pm ipz/\hbar}. \tag{17}
$$

They are orthogonal to each other with respect to the scalar product $\langle \psi | \phi \rangle = \int \psi^\dagger(z)\phi(z)dz$. For $\phi \equiv \psi$ this product gives the norm $\langle \psi | \psi \rangle$ which is conserved in the course of the (unitary) one-particle quantum dynamics in a fixed inertial frame of reference.

Another system of independent solutions of Eqs. (15) is presented by the eigenfunctions of the parity operator $\hat{P} = \beta \hat{P}_0$, which commutes with Dirac’s Hamiltonian $\hat{H}_D$ (but does not commute with $\hat{p}$); the matrix $\beta$ is the intrinsic parity. They are

$$
\psi_{+p, \uparrow}^E = \begin{pmatrix} \sqrt{\frac{E + mc^2}{2mc^2}} \cos \left(\frac{p_z}{\hbar} \right) \\ 0 \end{pmatrix}; \quad \psi_{+p, \downarrow}^E = \begin{pmatrix} 0 \\ \sqrt{\frac{E + mc^2}{2mc^2}} \sin \left(\frac{p_z}{\hbar} \right) \end{pmatrix},
$$

$$
\psi_{-p, \uparrow}^E = \begin{pmatrix} i \sqrt{\frac{E + mc^2}{2mc^2}} \sin \left(\frac{p_z}{\hbar} \right) \\ 0 \end{pmatrix}; \quad \psi_{-p, \downarrow}^E = \begin{pmatrix} 0 \\ -i \sqrt{\frac{E + mc^2}{2mc^2}} \cos \left(\frac{p_z}{\hbar} \right) \end{pmatrix}; \quad \psi_{-p, \uparrow}^E = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{18}
$$

the even solutions $\psi_{\uparrow}^E$ and $\psi_{\downarrow}^E$ correspond to the eigenvalue $+1$ of the parity operator, while the odd solutions $\psi_{\downarrow}^E$ and $\psi_{\downarrow}^E$ correspond to its eigenvalue $-1$ (it is evident that this system of independent solutions can be obtained from the plane-wave solutions (17), and wise versa).

Again, as in the nonrelativistic theory, the odd solutions become trivial in the limiting case $p = 0$. But such solutions are essential for any however small value of $p$. In this case the number of independent solutions to the four ordinary differential equations (see (14) and (15)) of the first order must be equal.
to the number of wave functions $\Phi_\uparrow$, $\Phi_\downarrow$, $\chi_\uparrow$ and $\chi_\downarrow$ which enter into these equations. Besides, in this case the current density $|\mathbf{J}|$ and average values of odd operators (see also Section 6) are proportional to $|\chi|$.

Thus, in passing from the Pauli theory to the Dirac one, the number of wave functions needed to describe the state of a particle increases by a factor of two, while the number of independent solutions for a given value of $E$ remains the same. In the nonrelativistic limit the Pauli equation for $\psi_\uparrow(z)$ is equivalent to two Dirac equations (13) for $\Phi_\uparrow(z;p)$ and $\chi_\uparrow(z;p)$. And the Pauli equation for $\psi_\downarrow(z)$ is equivalent to two Dirac equations (13) for $\Phi_\downarrow(z;p)$ and $\chi_\downarrow(z;p)$. From this it follows, in particular, that in this limit the Dirac bispinor $\Psi$ is compatible with the Pauli spinor $\psi$ only when all four its components are taken into account. That is, the nonrelativistic calibration implies that both the two-component spinors, $\Phi$ and $\chi$, are associated with the upper continuum of states of the Dirac particle.

Besides, both of them can be associated with the lower continuum of its states. The point is that the expression $p = \sqrt{E^2 - m^2c^2}/c$ is valid not only for the positive parameter $E$, but also for $-E$. Thus, we have also of the four independent solutions for the negative energy $-E$

$$
\Psi_{\pm E; \pm p, \uparrow}(z) = \left( \begin{array}{c} \mp z \\
2mc \pm z \\
0 \\
1 \end{array} \right) e^{\pm ipz/h}, \quad \Psi_{\pm E; \pm p, \downarrow}(z) = \left( \begin{array}{c} 0 \\
2mc \pm z \\
0 \\
1 \end{array} \right) e^{\pm ipz/h},
$$

(19)

which are orthogonal to each other and to the solutions (17).

So, both the systems of solutions, (17) and (19), are invariant with respect to the parity operator and, hence, each of them is complete. That is, all four components of each bispinor that enters into the system of solutions (17) describe the states of the Dirac particle with the positive energy $E$. Similarly, all four components of each bispinor that enters into the system of solutions (19) describe the states of the Dirac particle with the negative energy $-E$.

It should also be emphasized that each of the two systems (17) and (19) is invariant with respect to sign change before the (positive) parameter $p$. Thus, we may replace it by the parameter $p_z$ which can be both positive and negative. This means that the general solution to Eqs. (13) and (14) for the positive energy $E$ can be written in the form

$$
\Psi_{(\pm)}(z; p_z) = C_1(p_z)\Psi_{(\pm, \uparrow)}(z) + C_2(p_z)\Psi_{(\pm, \downarrow)}(z) + C_3(p_z)\Psi_{(\mp, \uparrow)}(z) + C_4(p_z)\Psi_{(\mp, \downarrow)}(z),
$$

(20)

where $E = \sqrt{c^2p_z^2 + m^2c^2}$; the coefficients $C_1(p_z), C_2(p_z), C_3(p_z)$ and $C_4(p_z)$ are determined by boundary conditions (see also Section 5). The corresponding time-dependent solution $\Psi_{(\pm)}(z, t)$, representing the superposition of four wave packets constructed from waves with $E \geq mc^2$, is

$$
\Psi_{(\pm)}(z, t) = \int_{-\infty}^{\infty} A(p_z)\Psi_{(\pm)}(z; p_z)e^{-iE(p_z)t/h},
$$

(21)

where the function $A(p_z)$ belongs to the Schwartz space. For example, we can take the Gaussian function $A(p_z) = \exp[(-z^2(p_z - p_0)^2 - i\bar{z}z_0)/2]$, where $p_0$, $\bar{z}$ and $z_0$ are given parameters.

In a similar way, we can write a time-dependent solution for energies in the region $[-mc^2, -\infty)$. The role of the lower continuum of states will be discussed in the next section. But before doing so we have to compare our solutions (17)-(19) with the standard ones.

Perhaps, the main difference is that in the standard approach a complete system of independent plane Dirac waves for a free particle is searched for a definite momentum $p_z = p$. In this case the equality $E^2 = c^2p_z^2 + m^2c^4$ is treated as an equation for the parameter $E$ with a fixed momentum $p_z$, and a searched-for complete system contains two independent solutions for the positive energy $E$ and two solutions for the negative energy $-E$. For example, a complete system presented in [4, 5] includes the solutions $\psi_{(\pm, \uparrow)}$, $\psi_{(\pm, \downarrow)}$, $\psi_{(\mp, \uparrow)}$ and $\psi_{(\mp, \downarrow)}$ in [6] a complete system consists of the solutions $\Psi_{(\pm, \uparrow)}$, $\Psi_{(\mp, \uparrow)}$, $\Psi_{(\pm, \downarrow)}$ and $\Psi_{(\mp, \downarrow)}$.

It is evident that these solutions (for them $C_2(p_z) = C_4(p_z) = 0$) allow one to build only the half of four wave packets needed to build the general nonstationary solution (21) for positive energies (see also Section 5). That is, none of these two systems represents a complete system of independent solutions to Eqs. (13) and (14) for a nonzero momentum. In particular, none of them allows one to obtain the even and odd solutions for any sign of energy. For $p_z \neq 0$, none of these two systems is invariant with
respect to the parity operator \( \hat{P} \). At the same time this requirement is necessary for a complete system of solutions to this problem, because \( \hat{P} \) commutes with the free Hamiltonian \( \hat{H}_D \).

Note that for \( p_z = 0 \) the parity operator \( \hat{P} \) represents the intrinsic parity \( \beta \), and the systems of solutions presented in [4, 5] become complete. The number of solutions in the systems (17) and (19) is halved in comparison with the case \( p_z \neq 0 \), while the number of solutions presented in [4, 5] remains the same.

For \( p_z = 0 \) the solutions (17) and (19) are reduced to two solutions, \( \Psi^{(E)}_{(0, \uparrow)} \) and \( \Psi^{(E)}_{(0, \downarrow)} \), for the positive energy and two solutions, \( \Psi^{-E}_{(0, \uparrow)} \) and \( \Psi^{-E}_{(0, \downarrow)} \), for the negative energy. Each of them is an eigenvector of the operator \( \beta \). In particular, the bispinors \( \Psi^{E}_{(0, \uparrow)} \) and \( \Psi^{E}_{(0, \downarrow)} \), in which only the component \( \Phi \) is nonzero, correspond to its eigenvalue \( +1 \); while the bispinors \( \Psi^{-E}_{(0, \uparrow)} \) and \( \Psi^{-E}_{(0, \downarrow)} \), in which only the component \( \chi \) is nonzero, correspond to its eigenvalue \( -1 \). As a consequence, both the standard approach and ours associate the large and small components of the Dirac bispinor with the positive and negative intrinsic parity, respectively. At the same time, these approaches quite differently assess the role of these two spinors in the Dirac theory.

According to our approach the Dirac bispinor in the standard representation obeys the requirements (b) and (c) of the nonrelativistic calibration. Thus, it represents the four-component probability amplitude that describes the state of a single relativistic fermion (or its antiparticle) with the positive energy. Doubling the number of components, in the passage from the Pauli theory to the Dirac one, is due to the change of the parity operator in the passage from the Galilean to Lorentzian symmetry (on the crucial role of the parity operator in the Dirac theory see, e.g., [7]). That is, this doubling is associated with the peculiarity of the description of the external, translational degrees of freedom of the Dirac particle, rather than with the appearance of its second internal degree of freedom.

4 On the role of the lower continuum of states

Now we have to dwell shortly on the question that concerns the transitions of a particle with the positive energy \( E \) into the lower continuum of states, due to a spontaneous emission of photons. In our approach we assume that they are impossible because they contradict the energy conservation law – the total energy of emitted photons cannot exceed \( E \). That is, states in the region \( E < 0 \) are inaccessible for the Dirac particle, and they have no physical meaning for it.

Of course, a sufficiently strong electric scalar potential can raise the states of the lower continuum to the upper one. But this fact does not at all mean that the states of the Dirac particle and its antiparticle are mixed with each other. Such a potential simply transforms the antiparticle states into the states of the very Dirac particle (such a situation arises in the Pauli paradox, which will be investigated in the next section).

In our opinion, the realistic Dirac theory should be based on the assumption that the Dirac particle with energy \( E \) is free in the infinitely remote spatial regions. That is, ‘realistic’ scalar potentials must be zero in the limit \( |r| \to \infty \). For example, the Coulomb and Coulomb-like potentials are realistic, while the parabolic potential of the harmonic oscillator taken as the electric potential \( \phi \) is not. We assume that the Dirac electron before the formation of a bound state with a positively charged nucleus is free and its total energy exceeds its rest energy. This electron can appear in a bound state due to the spontaneous emission of photons, and its minimum energy after radiation is strictly nonnegative.

5 The Klein tunneling and propagation of the electromagnetic wave in media with negative permittivity and permeability

Our next step is to address the Klein paradox. Let \( E \) be the particle energy, \( \mathcal{A}(r) = 0 \), and \( V(z) = c\phi(z) \) be a piecewise constant function: \( V(z) = V_0 = 0 \) for \( z < 0 \), and \( V(z) = V_r \) for \( z > 0 \); \( V_r \) is constant. Thus, in this problem the effective masses \( M(z) = m + [\epsilon - V(z)]/2c^2 \) and \( \mu(z) = [\epsilon - V(z)]/2c^2 \) of the heavy and light quasiparticles are piecewise constant functions too:

\[
M(z) = M_0 = m + \epsilon/2c^2, \quad \mu(z) = \mu_0 = \epsilon/2c^2, \quad z < 0; \quad M(z) = M_V = m + (\epsilon - V_r)/2c^2, \quad \mu(z) = \mu_V = (\epsilon - V_r)/2c^2, \quad z > 0.
\]
At the stage preceding the scattering event a particle is localized to the left of the potential step and moves toward the step strictly in the z-direction. All states of the particle are in the region $\epsilon > 0$ and obey Eqs. (5a), which can now be written in the form

$$\frac{\hbar^2}{2M_0} \frac{d^2 \Phi(z)}{dz^2} = \epsilon \Phi(z), \quad \left( \frac{\hbar^2}{2MV} \frac{d^2}{dz^2} + V_R \right) \Phi_R(z) = \epsilon \Phi_R(z), \quad \left( \chi^\uparrow \chi^\downarrow \right)_{l,r} = -\frac{i\hbar}{2cM_0M_V} \frac{\partial}{\partial z} \left( \Phi_i \right)_{l,r}$$

We first need to find general solutions for the spinors $\Phi$ and $\Phi_R$, and then to "sew" them at the point $z = 0$ with making use of the boundary conditions

$$\Phi_I = \Phi_R, \quad \frac{1}{M_0} \frac{d\Phi_I}{dz} = \frac{1}{MV} \frac{d\Phi_R}{dz},$$

which ensure the continuity of the spinors $\Phi$ and $\chi$ at the point $z = 0$.

As is seen, in this problem the equations for the components $\Phi_i$ and $\chi_i$, describing the Dirac particle with the 'spin up' in z-direction, are separated from the equations for the components $\Phi_r$ and $\chi_i$, corresponding to the particle with the 'spin down' in z-direction. Therefore it is sufficient to solve the problem for a particle with the 'spin up', with $\Phi_I = 0$ and $\chi_i = 0$. And, since this problem has already been solved in [1], we will dwell only on such aspects of this solution, which shed new light on the specifics of our approach to the Klein paradox.

Note that, as independent particular solutions in the interval $(-\infty, 0)$ where the particle is free, we may take the solutions $\Psi^{E}_{(p,\uparrow)}$ and $\Psi^{E}_{(p,\downarrow)}$ (in this Section we will consider only solutions with the positive energy, therefore the symbol $E$ (or $\epsilon$) will be omitted in the notation of these spinors and their components). For this purpose it is sufficient to substitute the quantities $M$, $\mu$ and $p$ in Exps. (17) by $M_0$, $\mu_0$ and $p_0$, respectively. Besides, for convenience let us pick out in these solutions the large components as well as the dependence on $z$. Namely, let

$$\Phi_{(\pm p,\uparrow)}(z) = \Phi_{(\pm p,\uparrow)}(z) = \chi_{(\pm p,\uparrow)}(z) = \chi_{(\pm p,\uparrow)}(z),$$

Then

$$\Psi_{(\pm p,\uparrow)}(z) = \Psi_{(\pm p,\uparrow)}(z) = \chi_{(\pm p,\uparrow)}(z) = \chi_{(\pm p,\uparrow)}(z).$$

Assuming, as in [1], that the amplitude of the wave impinging the step from the left is equal to the unit, let us write the general solution $\Phi_I$ of Eq. (22) for $\Phi$ in the interval $z < 0$ in the form

$$\Phi_I(z) = \Phi_{(p_0,\uparrow)} e^{ip_0z/\hbar} + B_I \Phi_{(p_0,\downarrow)} e^{-ip_0z/\hbar}, \quad p_0 = 2c\sqrt{\mu_0 M_0};$$

$B_I$ is constant.

What about the general solution $\Phi_R$ of Eq. (22) in the interval $z > 0$, a more detailed analysis is needed here (see [1]) because the energy domain $E > mc^2$ splits into three intervals in which solutions of Eq. (22) are qualitatively different. We will consider them separately.

5.1 Above-barrier scattering mode

We begin with the interval $\epsilon > V_0$. In this case $\epsilon' > V_0$ and the effective masses of the heavy and light quasiparticles are positive in the region $z > 0$. This means that this region of the repulsive potential is classically accessible for both quasiparticles. As a consequence, the general solution for $z > 0$ is

$$\Phi_R(z) = A_r \Phi_{(pv,\uparrow)} e^{ipVz/\hbar}, \quad p_V = 2c\sqrt{\mu_0 MV};$$

$A_r$ is an arbitrary constant; a particular solution $e^{-ipVz/\hbar}$ associated with the negative probability current density is excluded because the source of particles is located to the left of the potential step.

From the conditions (23) we find the amplitudes of the transmitted and reflected waves:

$$A_r = \frac{2}{1 + \alpha}, \quad B_I = \frac{1 - \alpha}{1 + \alpha}, \quad \alpha = \sqrt{\frac{\mu_0 M_0}{\mu_0 MV}}.$$
Thus, the transmission coefficient $T$ and the reflection coefficient $R$ are

$$T = \frac{J_{tr}}{J_{inc}} = \frac{4\alpha}{(1 + \alpha)^2}, \quad R = \frac{|J_{ref}|}{J_{inc}} = \left( \frac{1 - \alpha}{1 + \alpha} \right)^2; \quad (28)$$

$T = 0$ at the energy $\epsilon = V_r$ where the effective mass $\mu_V$ changes its sign. Thus, the solution of the stationary Dirac equation for energies $\epsilon > V_r$ is

$$\Psi_l(z) = \left( \begin{array}{c} \frac{1}{\sqrt{\frac{4\alpha}{M_0}}} \\
0 \end{array} \right) e^{ip_0z/h} + \frac{1 - \alpha}{1 + \alpha} \left( \begin{array}{c} \frac{1}{\sqrt{\frac{4\alpha}{M_0}}} \\
0 \end{array} \right) e^{-ip_0z/h}, \quad \Psi_r(z) = \frac{2}{1 + \alpha} \left( \begin{array}{c} \frac{1}{\sqrt{\frac{4\alpha}{M_0}}} \\
0 \end{array} \right) e^{ipVz/h}. \quad (29)$$

5.2 Total reflection

When $V_r - 2mc^2 < \epsilon < V_r$ the effective mass of the heavy quasiparticles in the region $z > 0$ is still positive: $M_V > 0$. But now this spatial region is classically forbidden for it. For the light quasiparticle $\epsilon' > V_r$ as before, but now $\mu_V < 0$. This means that the potential step acts on this quasiparticle as an attractive potential, and the region $z > 0$ is now classically accessible for it. As a consequence, the region $z > 0$ is classically inaccessible for the Dirac particle: solution for $z > 0$ has the form

$$\Phi_r(z) = A_r \Phi_{(pV, t)} e^{-\kappa z}; \quad p_V \equiv i\hbar \kappa = 2ic\sqrt{-\mu_V M_V}; \quad (30)$$

$A_r$ is an arbitrary constant.

Again, making use of the boundary conditions (23) for the solutions (24) and (30), we obtain

$$A_r = \frac{2}{1 + i\tilde{\alpha}}, \quad B_l = \frac{1 - i\tilde{\alpha}}{1 + i\tilde{\alpha}}, \quad \tilde{\alpha} = \sqrt{\frac{\mu_V M_0}{\mu_0 M_V}}. \quad (31)$$

In this case $T = 0$ because $|B_l| = 1$.

Thus, in the interval $V_r - 2mc^2 < \epsilon < V_r$ the searched-for solutions in both spatial regions are

$$\Psi_l(z) = \left( \begin{array}{c} \frac{1}{\sqrt{\frac{4\alpha}{M_0}}} \\
0 \end{array} \right) e^{ip_0z/h} + \frac{1 - i\tilde{\alpha}}{1 + i\tilde{\alpha}} \left( \begin{array}{c} \frac{1}{\sqrt{\frac{4\alpha}{M_0}}} \\
0 \end{array} \right) e^{-ip_0z/h}, \quad \Psi_r(z) = \frac{2}{1 + i\tilde{\alpha}} \left( \begin{array}{c} \frac{1}{\sqrt{\frac{4\alpha}{M_0}}} \\
0 \end{array} \right) e^{-\kappa z}. \quad (32)$$

5.3 The Klein tunneling

For $0 < \epsilon < V_r - 2mc^2$ – the Klein zone, not only $\mu_V < 0$ but also $M_V < 0$. That is, the potential step acts on both quasiparticles as an attractive potential. As a consequence, Exp. (23) for the (real) momentum $p_V$ is valid not only for $\epsilon > V_r$ but also for the Klein zone and, at the first glance, the solution (26) can be applied also to the Klein zone. However, this is not the case because the probability current density corresponding to this solution (wave with a positive phase velocity) is negative. This solution is not suitable because the source of particles is located to the left of the potential step. That is, in the Klein zone the phase velocity of the wave with the positive probability current density is negative in the spatial region $z > 0$:

$$\Phi_r(z) = A_r \Phi_{(-pV, t)} e^{-ipVz/h}; \quad (33)$$

$A_r$ is an arbitrary constant. With making use of the boundary conditions (23) one can show that the amplitudes $A_r$ and $B_l$ (see (20)) are determined by Exps. (24), as for the above-barrier mode. In the Klein zone Exps. (25) for the transmission and reflection coefficients are still valid.
In this zone, \( -p\nu/2M\nu c = +\sqrt{\mu\nu/M\nu} \), and hence the corresponding solution of the Dirac equation has almost the same form as for the above-barrier case:

\[
\Psi_t(z) = \begin{pmatrix} 1 \\ \frac{\mu}{\sqrt{M\nu}} \\ 0 \\ 0 \end{pmatrix} e^{ipz/\hbar} + \frac{1 - \alpha}{1 + \alpha} \begin{pmatrix} 1 \\ \frac{\mu}{\sqrt{M\nu}} \\ 0 \\ 0 \end{pmatrix} e^{-ipz/\hbar}, \quad \Psi_r(z) = \frac{2}{1 + \alpha} \begin{pmatrix} 1 \\ \frac{\mu}{\sqrt{M\nu}} \\ 0 \\ 0 \end{pmatrix} e^{-ip\nu z/\hbar}. \quad (34)
\]

It is evident that now, unlike the standard approach (see, e.g., [8]), not only \( T + R = 1 \), but also \( 0 \leq T \leq 1 \) and \( 0 \leq R \leq 1 \). Besides, both in the region \( z < 0 \) and in the region \( z > 0 \) the scattering particle has the same electrical charge \( e \) and full energy \( E \). Now there is no paradox. Moreover, as will be seen from the following, the Klein tunneling has an optomechanical analog.

5.4 Optomechanical analog of the Klein tunneling

Now we must show that there is an analogy between the Dirac particle moving in an external scalar electric field and the electromagnetic wave propagating in a dispersive medium with a relative permittivity \( \varepsilon_{\text{per}} \) and permeability \( \mu_{\text{per}} \) (here we are forced to slightly modify the traditional designation of these quantities) which, like the relative effective masses \( \tilde{M} \) and \( \tilde{\mu} \), can be both positive and negative. The point is that both phenomena are described by similar equations.

Indeed, if the scalar potential \( V = e\phi \) depends only on \( z \) and the particle moves along the \( OZ \)-axis, Eqs. (7) and (8) take the form

\[
\frac{d^2\Phi}{dz^2} - \frac{d\ln M}{dz} \cdot \frac{d\Phi}{dz} + k^2\tilde{\mu}\tilde{M}\Phi = 0, \quad \frac{d^2\chi}{dz^2} - \frac{d\ln \mu}{dz} \cdot \frac{d\chi}{dz} + k^2\tilde{\mu}\tilde{M}\chi = 0. \quad (35)
\]

These equations coincide in form with Eqs. (15) and (16) (see [9] p. 79) which describe the dynamics of the electric \( E_z = U(z) \exp(-i\omega t) \) and magnetic \( H_\phi = V(z) \exp(-i\omega t) \) components of the electromagnetic wave of the TE type, which moves along the \( z \)-direction in a layered medium inhomogeneous in this direction:

\[
\frac{d^2U}{dz^2} - \frac{d\ln \varepsilon_{\text{per}}}{dz} \cdot \frac{dU}{dz} + k^2\mu_{\text{per}}\varepsilon_{\text{per}} U = 0, \quad \frac{d^2V}{dz^2} - \frac{d\ln \varepsilon_{\text{per}}}{dz} \cdot \frac{dV}{dz} + k^2\mu_{\text{per}}\varepsilon_{\text{per}} V = 0; \quad (36)
\]

\( k = \omega/c \).

Thus, the equation for the spinor \( \Phi \), which describes the Dirac particle with the positive internal parity, coincides in form with the equation for the electromagnetic component of the electric wave; and the equation for the spinor \( \chi \), which describes a particle with negative internal parity, coincides with the equation for the magnetic components of the TE wave (see also [8]). In this case the relative effective mass \( \tilde{\mu} \) is an analogue of the relative dielectric permittivity \( \varepsilon_{\text{per}} \) and the relative effective mass \( \tilde{M} \) is that of the relative magnetic permeability \( \mu_{\text{per}} \).

Moreover, the relationship (22) between the spinors \( \Phi \) and \( \chi \) is similar to the relation (13b) (see [9] p. 79) which connects the electric and magnetic components of the electromagnetic wave:

\[
\chi^\dagger = -\sqrt{\frac{\mu_0}{M_0}} \cdot \frac{i}{k_0 M} \frac{d\Phi}{dz}, \quad V = -\frac{i}{k\mu_{\text{per}}} \frac{dU}{dz}. \quad (37)
\]

The factor \( \sqrt{\mu_0/M_0} \), which distinguishes these relations, reflects the fact that a complete analogy between the quantum ensemble of a massive Dirac particle and the electromagnetic wave associated with a massless photon can be expected only in the limit \( E \to \infty \). When \( E \) is finite, it is more correctly to compare the spinors \( \Phi \) and \( \chi \) with the electric and magnetic components of the electromagnetic field of a moving classical charged particle. In particular, in the reference frame in which the (massive) Dirac particle is at rest the spinor \( \chi \) is zero like the magnetic field of the (massive) classical particle.

Note that the key role in the Dirac theory and in classical electrodynamics is played by the products \( \tilde{M}\tilde{\mu} \) and \( \varepsilon_{\text{per}}\mu_{\text{per}} \); the Dirac particle can propagate in the external scalar electric field when \( \tilde{M}\tilde{\mu} > 0 \); the electromagnetic wave can propagate in a dispersive medium when \( \varepsilon_{\text{per}}\mu_{\text{per}} > 0 \). In both theories this is also true when both cofactors in these products are negative. The Klein tunneling in the region where
the (relative) effective masses of both quasiparticles are negative is analogous to the propagation of the electromagnetic wave in a medium with the negative dielectric permittivity and magnetic permeability (see [10–13]). In each case, the phase velocity of the wave and the corresponding energy transfer rate have opposite directions.

5.5 Wave packets in the Klein zone

Let’s consider the Klein tunneling by the example of the wave packet built of the stationary solutions obtained for Klein zone. We assume that at the initial instant of time the wave function \( \Phi(z, t) \) (the arrow \( \uparrow \) in the designations \( \Phi(z, t) \) and \( \chi(z, t) \) will be omitted further) that describes the subensemble of the heavy quasiparticle is a superposition of the stationary solutions \( \Psi(z; \epsilon) \) with the energy \( \epsilon \) that belong to the Klein zone. We also assume that at \( t = 0 \) the peak of this wave packet is at the point \( z = -a \) \((a > 0)\), far enough away from the potential step:

\[
\Psi(z, t) = \text{const} \cdot \int_{k_{\min}}^{k_{\max}} \Psi(z; k) G(k) \exp \left[ ika - i\epsilon(k)t/\hbar \right] dk,
\]

(38)

\( G(k) = \exp \left( -\frac{(k_{\max} - k_{\min})^2}{(k - k_{\min})(k_{\max} - k)} \right) \), if \( k = k_0 \in [k_{\min}, k_{\max}]; \epsilon(k) = \frac{\hbar^2 k^2}{(\sqrt{m^2 c^2 + \hbar^2 k^2} + mc)}; k_{\min,max} = \sqrt{\epsilon_{\min,max}(2mc^2 + \epsilon_{\min,max})}/\hbar c. \)

In the interval \( z < 0 \) this nonstationary state represents the superposition of the incident and reflected wave packets, while in the interval \( z > 0 \) we have only the transmitted wave packet. (By our approach, functions \( G(k) \) used for building a relativistic wave packet must belong to the Schwartz space. This ensures the existence of the average values of any degree of the momentum and position operators of the Dirac particle.)

Figs. 1-3 show the numerical results obtained for the squared modules of the wave functions \( \Phi(z,t) \) and \( \chi(z,t) \) for \( t = 0 \) (Fig. 1), \( t = 800 \) (Fig. 2) and \( t = 2000 \) (Fig. 3); \( V = 2.1, \epsilon_{\min} = 0.001, \epsilon_{\max} = V - 2.001, a = 100 \) (energy, time, and length are represented in the units of \( mc^2, \hbar/mc^2 \) and \( \hbar/mc \), respectively; the squared modules of the wave functions represented with an accuracy of the normalization multiplier). We note three salient features of the wave-packet dynamics: (i) the wave packet that describes the subensemble of heavy quasiparticles and the wave packet that describes the subensemble of light quasiparticles, both spread out with time; (ii) if \( z < 0 \) then the Dirac particle moves with a more probability as a heavy quasiparticle, while in the region \( z > 0 \), it moves with a more probability as a light quasiparticle (in the case of nonstationary states the total number of heavy

![Fig. 1](image-url) |\( |\Phi|^2 \) and |\( \chi|^2 \) as functions of \( z \) for \( t = 0 \): \( V = 2.1, a = 100, \epsilon_{\min} = 0.001, \epsilon_{\max} = V - 2.001 \)
and light quasiparticles is conserved); (iii) to the right of the potential step, wave packets constructed from waves with negative phase velocities move to the right along the \(OZ\) axis.

6 Effective hermitian operators in the space of spinors \(\Phi\)

As it follows from (5a), the small component \(\chi\) is uniquely determined by the large component \(\Phi\). This means that for any Dirac bispinor associated with a localized stationary state, the average value of any Hermitian operator can be calculated in the space of spinors \(\Phi\). For example, such states appear in the case of the Coulomb potential. As regards such non-relativistic potentials as a potential well with infinitely high walls as well as the parabolic potential that appears in the problem for a harmonic oscillator, they can not be considered in the Dirac theory as scalar electric potentials for which \(H_D\) has a discrete spectrum.
Let $\hat{O}_4$ be a hermitian operator defined in the space of Dirac bispinors, which has the form

$$\hat{O}_4 = \begin{pmatrix} a & \hat{g} \\ \hat{g}^\dagger & b \end{pmatrix}; \quad \hat{a}^\dagger = a, \quad \hat{b}^\dagger = b. \quad (39)$$

Then the operator $\hat{O}_2$ is its effective analogue defined in the space of spinors $\Phi$, if for any eigenvector $\Psi$ connected with an eigenvalue of the operator $\hat{H}_D$ of a discrete spectrum we have

$$\frac{\langle \Psi | \hat{O}_2 | \Phi \rangle}{\langle \Psi | \Phi \rangle} = \frac{\langle \Phi | \hat{O}_2 | \Phi \rangle}{\langle \Phi | \Phi \rangle} \equiv \int \phi^\dagger(r) \hat{O}_2 \phi(r) dr \int \phi^\dagger(r) \phi(r) dr \equiv \langle \hat{O}_2 \rangle; \quad (40)$$

$$\langle \Psi | \Phi \rangle = \langle \Phi | \Phi \rangle + \langle \chi | \chi \rangle.$$

By this definition the average value of the operator $\hat{O}_2$ describes the whole quantum ensemble of the Dirac particle. Besides, since the generalized Pauli equation (6a) for the spinor $\psi_k$ is the probability that the Dirac particle possesses the positive intrinsic parity. As it follows from Exp. (40), for odd operators the contribution of particles with the positive intrinsic parity is the operator $\hat{O}_2$ (see Section 4), the operators of the upper row of the matrix $\hat{O}_4$ describe the subensemble of heavy Schrödinger quasiparticles (Dirac particles with the positive intrinsic parity). Similarly, since the generalized Pauli equation (6a) for the spinor $\chi$ is associated with the lower row of the matrix, the operators of the lower row of the matrix $\hat{O}_4$ describe the subensemble of light Schrödinger quasiparticles (Dirac particles with the negative intrinsic parity).

Thus, considering the relation (5a) that links the spinors $\chi$ and $\Phi$, we have

$$\langle \Psi | \hat{O}_4 | \Psi \rangle = \langle \Psi | \hat{a} \Phi + \hat{g} \chi \rangle + \langle \chi | \hat{b} \Phi \rangle,$$

where the first summand represents the contribution of the positive intrinsic parity, while the second one is associated with the negative intrinsic parity.

It is evident that this expression, divided by $\langle \Psi | \Psi \rangle$, is reduced to the form (10) for

$$\hat{O}_2 = \left[ a + \frac{1}{2c} \left( \hat{g} \frac{1}{M} (\sigma \chi) + (\sigma \chi) \frac{1}{M} \hat{g}^\dagger \right) + \frac{1}{4c^2} \left( (\sigma \chi) \frac{1}{M} \hat{b} \frac{1}{M} (\sigma \chi) \right) \right] P_\Phi, \quad P_\Phi = \frac{\langle \Phi | \Phi \rangle}{\langle \Phi | \Phi \rangle + \langle \chi | \chi \rangle}. \quad (42)$$

where $P_\Phi$ is the probability that the Dirac particle possesses the positive intrinsic parity. As it follows from Exp. (42), for odd operators the contribution of particles with the negative intrinsic parity is the Hermitian conjugate of those with the positive intrinsic parity.

7 The effective energy operator

A more detailed analysis of Exp. (42) is possible only for particular operators. For example, for the velocity operator $\hat{v}_4 = c a$ we obtain the effective counterpart $\hat{v}_2 = \frac{c}{M} P_\Phi$. The Hamiltonian $\hat{H}_D$ gives another important example. In this case $\hat{a} = V + mc^2, \hat{b} = V - mc^2$ and $\hat{g} = \hat{g}^\dagger = c \sigma \hat{\pi}$. Thus, according to (40)–(42) we have $\hat{H}_2 = \hat{H}_D^+ + \hat{H}_D^-$ where the operators $\hat{H}_D^+$ and $\hat{H}_D^-$ describe the Dirac particle with the positive and negative intrinsic parity, respectively:

$$\hat{H}_D^+ = \left( \hat{K} + V + mc^2 \right) P_\Phi \equiv (\hat{H}_M + mc^2) P_\Phi; \quad \hat{H}_D^- = \left( \hat{K} + \hat{V}_- + \hat{E}_{res} \right) P_\Phi;$$

$$P_\Phi = \frac{1}{1 + \langle \phi | \phi \rangle}; \quad \hat{\kappa} = \sigma \pi \frac{1}{2M} \sigma \hat{\pi}; \quad \hat{V}_- = \sigma \pi \frac{V}{4Mc^2} \sigma \hat{\pi}; \quad \hat{\rho} = \sigma \pi \frac{1}{4Mc^2} \sigma \hat{\pi}; \quad \hat{E}_{res} = -mc^2 \hat{\rho} \quad (43)$$

For a more convenient comparison of the Dirac and Pauli theories let us move from the operator $\hat{H}_D$ to the operator $\hat{e}_4 = \hat{H}_D - mc^2$. Its projection is the operator $\hat{e}_2 = \hat{e}_2^+ + \hat{e}_2^-$, where $\hat{e}_+ = (\hat{K} + V) P_\Phi \equiv \hat{H}_M P_\Phi$ and $\hat{e}_- = (\hat{K} + \hat{V}_- + 2\hat{E}_{res}) P_\Phi$. With making use of useful equalities

$$\sigma \pi \frac{V}{M^2} + \left( 1 + \frac{V}{M^2 c^2} \right) \frac{i e \hbar}{M^2 c^2} \nabla \phi, \quad \nabla M = \frac{e}{2\hbar} \mathbf{E}, \quad \mathbf{E} = -\nabla \phi,$$

$$\hat{\pi} \times \hat{\pi} = \frac{i e \hbar}{c} \mathbf{H},$$

$$\mathbf{E} = \frac{e}{2\hbar} \mathbf{H}, \quad \nabla M = \frac{e}{2\hbar} \mathbf{E},$$

$$\sigma \pi \frac{V}{M^2} + \left( 1 + \frac{V}{M^2 c^2} \right) \frac{i e \hbar}{M^2 c^2} \nabla \phi, \quad \nabla M = \frac{e}{2\hbar} \mathbf{E}, \quad \mathbf{E} = -\nabla \phi,$$
we obtain

\[
\dot{\hat{\rho}} = \frac{1}{2Mc} \left( \hat{K} + \hat{\Delta}_H + 2\hat{\Delta}_E \right), \quad \dot{\hat{\nu}} = \frac{V}{2Mc^2} \left( \hat{K} + \hat{\Delta}_H \right) + \left( 1 + \frac{V}{Mc^2} \right) \hat{\Delta}_E,
\]

\[
\hat{K} = \hat{K} + \hat{\Delta}_H + \hat{\Delta}_E; \quad \hat{K} = \frac{1}{2M} \vec{\pi}^2, \quad \hat{\Delta}_H = -\frac{2\hbar}{2Mc} \sigma \mathbf{H}, \quad \hat{\Delta}_E = \frac{\hbar}{4Mc^2} (i\mathbf{E}\vec{\pi} + \sigma [\mathbf{E} \times \vec{\pi}]). \quad (44)
\]

As is seen, Exp. (44) for the operators \(\dot{\hat{\rho}}\), \(\dot{\hat{\nu}}\), and \(\dot{\hat{K}}\) contain non-Hermitian terms. However, since these operators themselves are Hermitian (see (43)), all their anti-Hermitian parts ultimately mutually compensate each other.

The representation of operators in the form (44) is convenient because the operators \(\hat{K}\), \(\hat{\Delta}_H\) and \(\hat{\Delta}_E\) in the nonrelativistic limit have clear physical meaning; \(\hat{K}\) is the operator of the kinetic energy of the Dirac particle with the positive intrinsic parity, which also includes its interaction with the vector potential; \(\hat{\Delta}_H\) is the operator describing the interaction of the magnetic moments of the particle with the external magnetic field; \(\hat{\Delta}_E\) is the operator that includes the Darwin term and the spin-orbit interaction. These operators are used also for determination of the projections of the corresponding operators for particles with the negative intrinsic parity.

Next, given the equality \(2Mc^2 - 2mc^2 + V = \epsilon\) (see (51)), we get

\[
\dot{\hat{e}}_2^+ = \left( \hat{K} + \hat{\Delta}_H + \hat{\Delta}_E + V \right) \hat{P}_\Phi, \quad \dot{\hat{e}}_2^- = \frac{\epsilon}{2Mc^2} \left( \hat{K} + \hat{\Delta}_H + 2\hat{\Delta}_E \right) \hat{P}_\Phi. \quad (45)
\]

Consequently

\[
\dot{\hat{e}}_2 = \left[ (1 + \frac{\epsilon}{2Mc^2}) \left( \hat{K} + \hat{\Delta}_H \right) + \left( 1 + \frac{\epsilon}{Mc^2} \right) \hat{\Delta}_E + V \right] \hat{P}_\Phi. \quad (46)
\]

What is important is that this analytical expression is exact for any energy \(\epsilon\).

8 Conclusion

As is shown, among different unitary representations of the Dirac theory, only one can support a consistent interpretation of this theory as a quantum theory of a single fermion. For choosing the required representation, we introduce the concept of a 'nonrelativistic calibration' of the relativistic quantum probability and show that only in the standard representation the Dirac bispinor admits a consistent interpretation as a four-component wave function, compatible in the nonrelativistic limit with a two-component wave function in the Pauli theory. The doubling of the number of components in the transition from the Pauli theory to the Dirac theory is explained by the differences in the description of the external (translational) degrees of freedom of the Dirac particle in the framework of the Lorentz and Galilean symmetries. That is, this doubling does not mean doubling the number of internal degrees of freedom of the Dirac particle.

It must be emphasized that, thanks to the "nonrelativistic calibration", the Dirac wave function, like the Pauli wave function, is determined to within a phase factor. Greater arbitrariness in its definition is unacceptable. This means, in particular, that all other representations cannot serve as a basis for the development of the quantum theory of a relativistic electron. And this fully applies to the Dirac theory in the FW representation.

On the basis of our approach we show that the Klein tunneling is analogous to the propagation of the electromagnetic wave in media with the negative dielectric permittivity and magnetic permeability. Besides, for one-particle operators, in the space of localized stationary states, we determine the corresponding effective operators which act in the space of the large component \(\Phi\), with taking into account of the contribution of the small component \(\chi\). The effective operator of energy is presented in a compact analytical form. Of course, it is desirable to generalize the concept of effective operators to the case of nonstationary localized states (wave packets), and also to the case of Lorentz scalar potentials.

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