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New Resolution of Klein Paradox by Modified Dirac Equations

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Abstract. We present a new resolution of the Klein paradox by considering the problem of electron incidence on a step potential barrier using modified Dirac equations (MDE). Contrary to the generally accepted interpretation, which is based on the Dirac equation (DE) and predicts electron tunneling through an infinitely high barrier, our calculations show that tunneling is impossible if the electron kinetic energy is less than the barrier height. We propose to investigate MDE as an alternative DE relativistic quantum mechanical equation for spin ½ particles

Keywords: relativistic electron, potential barrier, Modified Dirac Equation, tunnelling, new Hamiltonian, new energy-momentum relation, antiparticles, negative energy, theory of holes

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1. Introduction

In recent years, a new relativistic theory of particle-electromagnetic field interaction has been developing [1-6]. This theory successfully addresses some of the difficulties of the traditional theory of electromagnetism in describing the behavior of charged particles in an electric field at high potentials. One notable problem, mentioned in [5] and studied in [6], is the inability of traditional theory to correctly describe the passage of a relativistic particle through a high potential barrier. The problem is that relativistic quantum mechanical equations give a sinusoidal wave function for a particle in the barrier region, which contradicts the established exponentially decreasing probability of tunneling through the barrier; moreover, this wave function do not transform into exponentially decreasing functions of the Schrödinger equation even in the non-relativistic limit. The source of this problem is the generally accepted relation between energy and momentum, which gives the real momentum of a particle inside a high-barrier region, whereas according to the law of conservation of energy, the momentum of a particle there must be imaginary. This problem was resolved in [6] using a new energy-momentum relation and, based on it, a modified Klein-Fock-Gordon equation for a spinless particle. The approach yielded the expected imaginary momentum for the particle and exponentially decreasing, rather than sinusoidal traveling wave functions inside the barrier. Consequently, plausible results were obtained, that the probability of tunneling exponentially decreases with the increase of the height and length of the barrier, and therefore a relativistic spinless particle cannot pass through an infinitely high barrier. In this paper, a similar problem is examined for the electron, whose behavior in the high-barrier region is the subject of the Klein paradox.

The Klein paradoxes, known for more than 90 years [7], arise when using Dirac equation (DE) to study scattering of electron on a step potential barrier (Fig.1) of the form

$$U=\begin{cases}0 & \text{at} \quad x<0\\ U_0<0 & \text{at} \quad x>0\end{cases}. \tag{1}$$

When considering this problem in the non-relativistic limit, the Schrödinger equation provides a well-known and plausible result: an electron is reflected from the barrier when its energy is less than the barrier height, and at an energy greater than the barrier height, there are non-zero probabilities of both reflection and passage. However, when solving this problem using the DE, some paradoxical results emerge. For example, it turns out that an electron can pass through an infinitely high barrier (Klein tunneling). Thus, Klein tunneling is a relativistic quantum mechanical theoretical result that arises from the DE for the electron.

2. Solutions of Dirac equation

The stationary DE, which determines the 4-component wave function ψ of an electron, in the electrostatic potential *U*, can be written as

$$\left[E - eU + ic\hbar\boldsymbol{\alpha}\frac{\partial}{\partial\mathbf{r}} - mc^2\beta\right]\psi = 0 \ , \tag{2}$$

where *E* is the energy of the electron, m and $e < 0$ are the mass and charge of the electron, *c* is the speed of light, $\hbar$ is Planck's constant, $\boldsymbol{\alpha}, \beta$ are the Dirac matrices. The DE, as is known, is constructed on the bases of the relativistic Hamiltonian

$$H = eU + \sqrt{(cP)^2 + \left(mc^2\right)^2} \tag{3}$$

by replacing the quantities of energy *E* and momentum ***P*** with the corresponding operators $i\hbar\partial/\partial t$ and $-i\hbar\partial/\partial\mathbf{r}$ and linearizing the radical using 4x4 matrices $\boldsymbol{\alpha}$ and β as coefficients with partial derivatives [8]. The result is a system of 4 linear first-order partial differential equations, which in the stationary case leads to equation (2) for the 4-component wave function. Two of these functions correspond to two opposite directions of spin for a particle with positive energy, and the other two correspond to two opposite directions of spin for an antiparticle, having the opposite sign of the charge and negative energy.

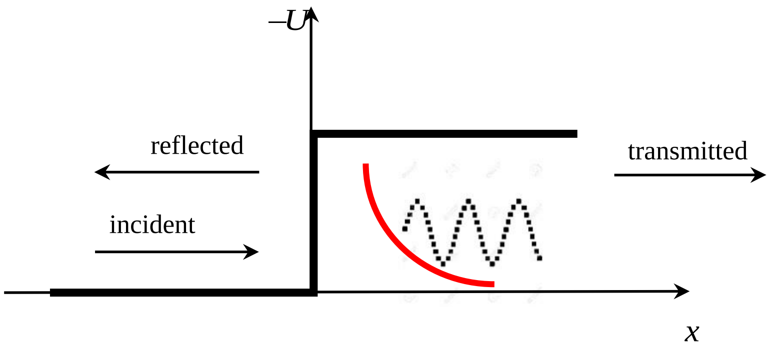

Fig. 1. Sketch of a step potential barrier. The arrows indicate the direction of propagation of the incident, reflected, and transmitted wave functions. The solid red curve shows the exponentially decreasing amplitude of the wave function calculated using the Schrödinger equation, the dotted black curve shows the sinusoidal real (or imaginary) part of the wave function calculated using the Dirac equations.

For the problem under consideration, solutions to Eq.2 in the region $x < 0$ represent two counter propagating waves, incident and reflected, with momentums $\pm p = \pm (E^2 - mc^2)^{1/2}$. In the region $x > 0$, there is one transmitted wave $T\exp(iPx)$, the momentum P of which is determined from the well-known energy-momentum relation

$$(cP)^2 = (E - eU)^2 - \left(mc^2\right)^2 = E^2 - \left(mc^2\right)^2 - 2EeU + (eU)^2. \qquad (4)$$

From the requirement of continuity of the wave function at $x = 0$, the following reflection R and transmission T coefficients are obtained:

$$R = \frac{1-\eta}{1+\eta} \qquad T = \frac{2\sqrt{\eta}}{1+\eta} \quad , \qquad (5)$$

where

$$\eta = \frac{P}{p}\frac{E+mc^2}{E-U_0+mc^2} = \frac{\sqrt{(E-eU_0)^2-\left(mc^2\right)^2}}{\sqrt{E^2-\left(mc^2\right)^2}}\frac{E+mc^2}{E-eU_0+mc^2} \ . \qquad (6)$$

At a small barrier height, when $eU_0 < E - mc^2$, the momentum P and the parameter η are real and from (5), (6) it follows that the electron can either be reflected from the barrier with probability $|R|^2$, or pass through the barrier with probability $|T|^2$. For a larger eU_0, when $E + mc^2 > eU_0 > E - mc^2$, the momentum P and the parameter η are imaginary, which gives for the probability of reflection $|R|^2 = 1$, and for the probability that the electron will be detected inside the barrier at a distance x – an exponentially decreasing expression $|T|^2\exp(-2|P|x/\hbar)$. Thus, at $E + mc^2 > eU_0 > E - mc^2$, the electron is reflected from the barrier.

However, at higher values of eU_0, the momentum P again becomes real and the wave function at $x > 0$ becomes a sinusoidal traveling wave, indicating the passage of the electron through the barrier. Moreover, as eU_0 tends to infinity, the parameter η and the transmission coefficient T do not tend to zero, which means that there is a non-zero probability of an electron passing through an infinitely high barrier (it is believed that, since the group velocity of the electron $v_g = dE/dP = c^2P/(E - eU_0)$ is negative, then for P in (6) one should take a negative sign, which gives $\eta > 0$ and T tending to a positive number).

The traditional resolution of such anomalous tunneling uses the concept of particle-antiparticle pair production in the context of quantum field theory. However, anomalous tunneling can also occur at a barrier profile with a non-zero wall thickness [9], therefore, Klein tunneling is a property of relativistic wave equations and may not associated with the birth of new particles [10]. Other models investigating the Klein paradox propose a single-particle approach: replacing the physical process of pair production by virtual negative energy scattering under the barrier [11], and using equations that include the second derivative with respect to time [12]. Thus, the current consensus regarding Klein tunneling posits that an electron can pass through an infinitely high potential barrier.

However, this theoretical result lacks experimental confirmation and is, in fact, scientific speculation. The result is doubtful since the electron momentum P, according to equation (4), is a real quantity that results in a sinusoidal traveling (rather than an exponentially decaying) wave function in the barrier region $x > 0$. This wave function, in the nonrelativistic limit, does not converge to the exponentially decaying wave function of the Schrödinger equation. Also, this tunneling phenomenon contradicts the result for a spinless particle, which, as discussed above, cannot pass through an infinitely high barrier. Such radically different behavior between an electron and a spinless particle has no reasonable explanation.

3. Solutions of modified Dirac equation

In this paper we propose a new solution to the Klein paradox, where such tunneling turns out to be impossible. The problem is solved by using, instead of the DE, another, modified Dirac equation (MDE), which is written as:

$$\left[E + ic\hbar\boldsymbol{\alpha}\frac{\partial}{\partial\mathbf{r}} - \left(mc^2 + eU\right)\beta\right]\psi = 0 \ . \tag{7}$$

This equation is constructed from the expression of a new Hamiltonian

$$H = \sqrt{\left(cP\right)^2 + \left(mc^2 + eU\right)^2} \tag{8}$$

in similar way as (2) is constructed from (3). The Hamiltonian (8) appeared first in scalar theories of gravity [13, 14], giving a new energy-momentum relation (10), which was used in the New theory of electromagnetic interactions [1-6]. The solutions of MDE (7) are 4-component wave functions ψ of a particle with spin ½.

Solving equations (7) in a similar to (3) way, we arrive at the same expressions (5) for the reflection and transmission coefficients, but with a new formula for the parameter η, written as

$$\eta = \frac{P}{p}\frac{E + mc^2}{E + mc^2 + eU_0} = \frac{\sqrt{E^2 - \left(mc^2 + eU_0\right)^2}}{\sqrt{E^2 - \left(mc^2\right)^2}}\frac{E + mc^2}{E + eU_0 + mc^2} \ . \tag{9}$$

Here P is determined from equation

$$\left(cP\right)^2 = E^2 - \left(mc^2 + eU\right)^2 = E^2 - \left(mc^2\right)^2 - 2mc^2eU - \left(eU\right)^2 \ , \tag{10}$$

which is obtained from (8). The expression (9) shows that (as well as in Eq.6) the parameter η becomes imaginary, and the probability of reflection $|R|^2 = 1$ when $eU_0 > E - mc^2$. However, in contrast to Eq.6, the momentum P and the parameter η remain imaginary also at any higher values of eU_0, i.e. the wave function in the region $x > 0$ for large values of eU_0 is an exponentially decreasing, rather than a sinusoidal traveling wave, as in the previous case. Therefore, tunneling through the barrier is not possible here. Thus, consideration of the problem of electron scattering on a step potential barrier within the framework of MDE (7) provides a fundamentally new solution to the Klein paradox, which rejects the possibility of tunneling through high barriers.

From equations (4) and (10), it is seen that a significant difference between them is the presence of a linear with respect to E term on the right-hand side of (4), which is absent in (10). Due to this term, positive and negative energy values ±E give different momentums. Therefore, for completeness, it is necessary to account for both signs of energy, which necessitates the introduction of negative energies in the DE.

However, in the new relation (10), there is no linear term, so the magnitude of the momentum does not depend on the sign of the energy. Both positive and negative energies ±E correspond to the same value of momentum, and therefore there is no need to introduce negative energies. Hence, the 4-line wave function in the MDE can be interpreted such that two components correspond to two opposite spin directions and positive momentum for a particle, and the other two components correspond to two opposite spin directions and negative momentum for the same particle (having positive energy).

Thus, the MDE implies that the particle's energy is always positive. This is consistent with the results of the new classical theory [5], which shows that the potential energy of a charged particle in an electrostatic potential has a minimum value of $-mc^2$, i.e. the total energy of the particle (including the rest energy mc^2) is always positive.

As it known, from the DE follows the possibility of the existence of antiparticles with opposite charge sign and negative energy [8]. To circumvent the difficulty of negative energy and predict the existence of real antiparticles with positive energy, Dirac proposed the concept of "holes" in the infinite number of electrons with negative energy, which occupy almost all negative states and associated the vacant states - "holes" with protons [15] (later holes were considered as positrons). However, this concept has faced many problems and criticism. MDE describes both particles and antiparticles with positive energy similarly, by rejecting the possibility of negative energies, so Dirac's concept of holes, becomes unnecessary.

4. Conclusions

We presented a modified Dirac equation (MDE) based on the new Hamiltonian (8) as a relativistic quantum mechanical equation for spin ½ particles. MDE has the advantages over the DE, it describes both particles and antiparticles with positive energies, whereas the DE describes antiparticles with negative energies, which do not exist in nature. In the nonrelativistic limit, solutions of the MDE transform into the corresponding solutions of the Schrödinger equation, while solutions of the DE can remain significantly differing from those of the Schrödinger equation.

Applying the MDE to the problem of electron scattering on a step potential barrier reveals that the electron's momentum inside the barrier is imaginary, leading to a plausible exponentially decreasing wave function inside the barrier, rather than the sinusoidal traveling wave function, resulting from the DE. As a result, it follows that an electron cannot pass through the barrier and is reflected if its kinetic energy is less than the height of the barrier. Especially, an electron cannot pass through an infinitely high barrier. MDE is based on a new Hamiltonian (8), which yields a new energy-momentum relation (10). The theoretical arguments discussed above support this new relation rather than the traditional relation (4), and therefore favor MDE over DE. Further research is needed on various issues within the MDE framework.

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