The Klein paradox and the zitterbewegung of an electron in a field with a constant scalar potential

S. V. Vonsovskii and M. S. Svirskii

Institute of Metals, Ural Branch, Russian Academy of Sciences, Ekaterinburg; Chelyabinsk State Pedagogical Institute (Submitted 26 October 1992; resubmitted after revision 3 February 1993) Usp. Fiz. Nauk 163, 115–118 (May 1993)

The zitterbewegung of an electron in the case of a field with a constant nonzero scalar potential is examined. The relationship of the average velocity of the particle and its momentum is discussed, and also the relation between the energy and the scalar potential. It is shown that taking this relationship into account enables one to resolve the well-known Klein paradox in Dirac's relativistic quantum theory of the electron.

1. INTRODUCTION

As is well known, already in 1929 Klein¹ in solving the Dirac² relativistic equation formulated a paradox which, as has been noted, for example, in Ref. 3 (see also § 35 in Ref. 4, § 5 in Part 2 of Ref. 5 and in Ref. 6) is a famous example of the difficulties of the Dirac quantum theory of a relativistic electron. This paradox refers to the problem of explaining the process occurring in the incidence of a free electron wave with positive energy on a rectangular potential step of height U_0 . Using in this case the usual condition of continuity of the wave function at the potential barrier we arrive for a sufficiently large value of U_0 obeying the condition

$$U_0 > E + m_0 c^2,$$
 (1)

where E is the energy, m_0 is the rest mass of the particle and c is the velocity of light, at the paradoxical conclusion that the electron flux reflected from the potential step exceeds the incident flux. The unusual nature of this conclusion is characterized, for example, by the authors of Ref. 3 in the following words: "The picture ceases to correspond to reality".

It seems to us that the Klein paradox can be resolved if we take into account the characteristic for the Dirac theory² "uncoupling" of the well-known in classical mechanics connection between the momentum and the velocity of a particle. The first one to call attention to this circumstance was Breit⁷ (see also p. 550 in the collected works of Pauli⁸). According to the Dirac theory the operator v_z of the projection of the velocity of the particle on its momentum (we assume that the z axis is chosen along the momentum) is proportional not to the operator p_z of the projection of the momentum (which would correspond to the equality $p_z = mv_z$ of classical mechanics), but to the Dirac matrix α_z (cf., for example, formula (24) in § 69 in Ref. 2):

$$v_z = c\alpha_z. \tag{2}$$

From (2) it follows that the operator v_z has the eigenvalue $\pm c$, since the eigenvalues of the Dirac matrix are equal to

 ± 1 . This result which, at first glance, contradicts the fact that the electrons observed in practice have velocities whose magnitude is smaller that the velocity of light, led to the concept of the zitterbewegung of the electron. This was first shown by Schrodinger⁹ (see also Refs. 5, 8 and others). The "jittery" part of the motion of a free electron can be easily obtained if one integrates the quantum equation of motion for the projection of the electron velocity, i.e., according to (2) for the matrix α_z . This equation of motion has the form

$$i\hbar\dot{\alpha}_z = \alpha_z H_0 - H_0 \alpha_z, \tag{3}$$

where $2\pi\hbar$ is the Planck constant, the dot above the line denotes a derivative with respect to the time t, and H_0 is the Hamiltonian of the free particle (cf., below formula (6)). It can be easily shown (cf., for example, § 70 from Ref. 2) that the integration of (3) yields

$$\alpha_{z} = \frac{1}{2} i \hbar (\dot{\alpha}_{z})_{0} e^{-2iH_{0}t/\hbar} H_{0}^{-1} + c p_{z} H_{0}^{-1} = \alpha_{z, \text{osc}} + \alpha_{z, \text{const}},$$
(4)

where $(\dot{\alpha}_z)_0$ is a constant equal to the value of $\dot{\alpha}_z$ for t=0. Thus, according to (4) in the case of free motion the projection of the velocity of the electron on the direction of its momentum is equal to the sum of the oscillating $\alpha_{z,osc}$ and the constant $\alpha_{z,const}$ parts.

In Ref. 10 we have shown that the zitterbewegung from (4) corresponds to the representation of the steady state of the electron in the form of a superposition of two eigenstates of the operator (2) with the eigenvalues +c and -c. Here the average value of the operator (2) is given by the equation

$$\bar{v}_z = \frac{c^2 p_z}{E}.$$
 (5)

This expression coincides, according to (2) and the second term in the right hand side of (4) with the eigenvalue of the constant part of the velocity operator $v_{z,const}$. From (5) we can also see that the directions of the average velocity and the momentum coincide only in the stationary states of positive energy. In states of negative energy they according

to (5) are antiparallel. This last circumstance is what leads one, as will be shown below, to a resolution of the Klein paradox. However, at first one should examine how the zitterbewegung of a particle in a field with a constant scalar potential will be altered.

2. THE ZITTERBEWEGUNG OF PARTICLE IN A FIELD WITH A CONSTANT SCALAR POTENTIAL

In the case of motion of a particle with rest mass m_0 in a field with a constant nonzero scalar potential U_0 the Dirac Hamiltonian has the form (cf., formula (23) in § 69 of Ref. 2)

$$H = c\alpha_z p_z + \beta m_0 c^2 + U_0 = H_0 + U_0, \qquad (6)$$

where α_z and β are the Dirac matrices, and H_0 is the Hamiltonian for free motion, utilized above in (3). Thus, in the presence of a constant scalar potential an equality of the form of (4) holds for α_z in which one should replace H_0 by $H - U_0$. Therefore instead of the second term in the right hand part of (4) we shall have

$$\alpha_{z,\text{const}} = c p_z (H - U_0)^{-1}, \tag{7}$$

and in place of (5)

$$\bar{v}_z = \frac{cp_z}{E - U_0}; \tag{8}$$

where E is the eigenvalue of the Hamiltonian (6), which is equal to

$$E - U_0 = \pm (m_0^2 c^4 + c^2 p_z^2)^{1/2}.$$
 (9)

It is not difficult to convince oneself of the validity of (9) by squaring the expression $H-U_0$ from (6) and using the relationships $\alpha_z\beta+\beta\alpha_z=0$ and $\alpha_z^2=\beta^2=1$ which are satisfied by the Dirac matrices (cf., Ref. 2). It can be seen from (8) and (9) that when in the right hand side of (9) the plus sign appears the quantities \bar{v}_z and p_z have the same sign, while in the case of a minus sign these vectors are antiparallel. From formulas (8) and (9) it also follows that the dependence of the average velocity and its root-mean-square indefiniteness $[(\Delta v_z)^2]^{1/2} = [c^2 - (\bar{v}_z)^2]^{1/2}$ on p_z and m_0 have externally the same appearance as the dependence (5), and the dependence

$$[(\Delta \overline{v_z})^2]^{1/2} = c \, \frac{m_0}{m},\tag{10}$$

where m is the mass of the moving electron, which were first established by us in Ref. 10 (see there formula (12)) for the case of free motion.

From the normalization condition W(c) + W(-c) = 1(W(c) is the probability of the state), in which the eigenvalue of the velocity is equal to +c, while W(-c) is the probability of the state where this value is equal to -c, and also from the preservation of the dependence of the average value of the velocity \overline{v}_z on p_z and m_0 (it is related to the probabilities by the relationship $\overline{v}_z = c(W(c) - W(-c))$) it follows that in a field with a constant scalar potential the same dependences are preserved externally which were obtained in formulas (9) and (10) for the first time in our paper of Ref. 10 for the probabilities in the case of free motion. This agrees with the fact that in correspondence with gauge invariance the addition to the Hamiltonian of a constant potential is equivalent to multiplying the wave function by the phase factor $e^{-iU_0t/\hbar}$ and, consequently, this should not alter the probabilities of the states the superposition of which forms in accordance with Ref. 10 the steady state of a particle the motion of which is described by the Dirac equation.

3. RESOLUTION OF THE KLEIN PARADOX

We denote the region of space with z < 0 in which the potential is U=0 by the number 1, and the region z>0 in which the potential is $U = U_0 > 0$, by the number 2. Then in region 1 the positive energy according to (9) is equal to $E = (m_0^2 c^4 + n + c^2 p_{1,z}^2)^{1/2}$ while in region 2 it is determined by the expression (9) with the momentum $p_{2,z}$. As the particle moves in region 1 the inequality $p_{1,z}^2 > 0$, holds which means that the momentum $p_{1,z}$ is real. At the same time the energy which has just been introduced above satisfies the inequality $E > m_0 c^2$. Together with the condition (1) this is equivalent to the inequality $U_0 > 2m_0c^2$ and, as is well known from the Dirac theory, the energy gap between levels with negative and positive energies is equal to $2m_0c^2$. Therefore this inequality means that the potential energy U_0 is so great that under its influence the energy levels which for U=0 were negative can now under the influence of U_0 be elevated and turn out to be in the region of positive energies where $E > m_0 c^2$. Correspondingly the energy in the region 1 (cf., formula (9) in the text above) and the energy in the region 2: $E = U_0 - (m_0^2 c^4 + c^2 p_{2,z}^2)^{1/2}$, which is obtained from (9) in the case that the minus sign appears in its right-hand side, can turn out to be equal. Then in the case when the inequality (1) is satisfied the quantity $p_{2,z}^2$ turns out to be positive and, consequently, is real. Therefore in the case of such a positive energy, for which both $p_{1,z}$ and $p_{2,z}$ are real, a transition from region 1 to region 2 is possible.

We now examine the average value of the projection of the velocity on the z axis in region 1 and in region 2. If the flux of the particles is directed from region 1 into region 2, then in the region 1 the inequality $\bar{v}_{1,z} > 0$ should hold. In the same region 1, where the electron moves freely, the equality $\bar{v}_{1,z} = c^2 p_{1,z}/E$ should hold in accordance with (5). In the case of a positive energy E according to this equality, and also if the inequality for the average velocity just stated above, holds, the inequality $p_{1,z} > 0$ should also hold. Thus in region 1 the momentum is parallel to the average velocity of the particle and, just as the average velocity, is directed from region 1 into region 2.

It follows from (8) and (9) that in region 2 $\overline{v}_{2,z} = \pm c^2 p_{2,z} (m_0^2 c^4 + c^2 p_{2,z}^2)^{-1/2}$. Since under the conditions of the Klein paradox positive energy levels are considered which arose from negative ones (for U=0), due to the sufficiently great value of U_0 , one should in accordance with (9) retain the minus sign in the right-hand side of the expression for $\overline{v}_{2,z}$ given above. If we now assume that in going from region 1 into region 2 the direction of the momentum is preserved, i.e., $p_{2,z} > 0$, then we obtain $\overline{v}_{2,z} < 0$. This means that in region 2 the flux of particles is directed not from region 1 into region 2, but conversely from region 2 into region 1 which is what leads to the Klein paradox (cf., Ref. 2).

It seems to us that it is possible to resolve the Klein paradox if we do not from the outset assume that the direction of the momentum $p_{2,z}$ coincides with the direction of the momentum $p_{1,z}$. Such an assumption, which is commonly used, corresponds to nonrelativistic quantum mechanics according to which in the case of a plane wave with the propagation vector k and the momentum $p = \hbar k$ the direction of the flux density of the particles coincides with the direction of the momentum. Therefore in nonrelativistic quantum mechanics the flux of the particles from region 1 into region 2 corresponds to the same sign of the components $p_{1,z}$ and $p_{2,z}$. But in the Dirac relativistic theory (cf., formulas (2), (5) and (9)) there is no analogous connection between the flux densities and the momentum. In this theory, as can be seen for example from (5), for a negative energy E < 0 the signs of the quantities \bar{v}_z and p_z turn out to be opposite. Therefore at the potential step there can occur a change not only of the magnitude but also of the direction of the momentum vector. Therefore if when the inequality $p_{1,z} > 0$ holds one assumes $p_{2,z} < 0$ then from the equality given above in the text for the average velocity in region 2 it follows that $\bar{v}_{2,z} > 0$. In this case the particle fluxes in region 1 and region 2 turn out to be parallel and the Klein paradox does not arise. It is also not difficult to convince oneself that the requirement of the continuity of the solutions of the Dirac equations at the boundary of the potential step leads to the equations

$$A_{\rm inc} = \frac{1}{2} (1+r) D_{\rm tr}, \quad B_{\rm refi} = \frac{1}{2} (1-r) D_{\rm tr},$$

where A_{inc} , B_{refl} and D_{tr} are the amplitudes of the plane waves incident on the step, reflected from it and transmitted through it, while the quantity r is given by

$$r = \frac{p_{2,z}}{p_{1,z}} \left(E + m_0 c^2 \right) \left[U_0 + \left(E + m_0 c^2 \right) \right]^{-1}.$$

Correspondingly the equation $\bar{v}_{z,inc} = |\bar{v}_{z,refl}| + \bar{v}_{z,tr}$ holds from which for $\bar{v}_{z,tr} > 0$ it follows that $|\bar{v}_{z,refl}| < \bar{v}_{z,inc}$. Thus, the picture is reestablished which corresponds to the usual concepts concerning processes of reflection of a flux of particles from the boundaries of a potential step and transmission through it.

4. CONCLUSIONS AND DISCUSSION

In the present paper results are generalized of the investigation of Ref. 10 to the case of a particle in a field with a constant nonzero scalar potential. The discussion that has been presented enabled us to resolve in a natural manner the Klein paradox. In this connection it is useful to make the following remark. Until now in the physics literature, as a rule, an opinion has been stated that the conclusion following from the Dirac theory concerning the equality of the eigenvalues of the velocity of the operator of an electron corresponding to values $\pm c$, i.e., equal in mag-

nitude to the velocity of light is devoid of physical sense. However it seems that the results, obtained by us both in section 4 of Ref. 10 and also in the present article, indicate the deep physical sense of this conclusion of the Dirac theory. Also one should note that the conclusions made in Ref. 10 and here refer not only to the truly relativistic rapidly moving particles, but also to particles with average velocities small compared with the velocity of light (this case can be realized by going over into an appropriate inertial reference system). For such "nonrelativistic" particles the special theory of relativity also leads to conclusions essentially different from the classical Newtonian mechanics, in particular to a conclusion concerning the existence of a rest energy. In this connection we note that we in Refs. 11, 12, and also other authors (Refs. 13-15), have established within the framework of the band theory of solids the existence of zitterbewegung also for an essentially nonrelativistic electron.

In the case of free motion the role of the rest energy manifests itself in the fact that, as we have shown in formula (12) of Ref. 10, the root-mean square indefiniteness of the projection of the electron velocity along the momentum is equal to $(m_0c^2)c/E$. Correspondingly this indefiniteness is maximum and equal to c in the rest system where $E = m_0c^2$. In a reference system where the electron energy significantly exceeds its rest energy this indefiniteness tends to zero, while the electron velocity tends to the velocity of light.

According to (2), (8) and (9) in a field with a constant scalar potential the indefiniteness of the component of the velocity along the momentum is determined by the equation

$$[\overline{(\Delta v_z)^2}]^{1/2} = \frac{m_0 c^2}{|E - U_0|} c.$$

Thus also in this case the role of the rest energy is made apparent. For $U_0=0$ this expression goes over into formula (12) of Ref. 10 which we have discussed earlier. When the condition (1) holds the expression for the indefiniteness under discussion takes on the form just indicated above, from which it follows that under the conditions examined in connection with the Klein paradox as U_0 increases the root-mean-square indefiniteness of the component of the velocity along the momentum decreases.

In conclusion we note that the concept proposed by us in Ref. 10 and developed in the present article of a stationary state of a particle in the form of a superposition of eigenstates of the velocity operator with the eigenvalues of this operator equal to $\pm c$ is in complete accord with the general principle of the superposition of states of quantum mechanics. This reflects the inner motion of particles with a nonzero rest mass in accordance with relativistic quantum mechanics, and this enables one to gain a better understanding of the nature of particles the motion of which obeys both the laws of quantum mechanics and the laws of the special theory of relativity.

¹O. Klein, Z. Phys. 53, 157 (1929).

²P. A. M. Dirac, The Principles of Quantum Mechanics, 3rd ed., Clar-

endon Press, Oxford, 1947 [Russ. transl., Fizmatgiz. M., 1960].

- ³J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics*, McGraw-Hill, N.Y., 1964 [Russ. transl., Nauka, M., 1978].
- ⁴Ya. I. Frenksl', *Wave Mechanics*, Part 2 (In Russian), ONTI, L., M., 1934.
- ⁵W. Pauli, Die Allgemeinen Prinzipien der Wellenmechanik, Handbuch der Physik, 2 Aufl., Band 24, I. Teil [Russ. transl., Gostekhizdat, M., L., 1947].
- ⁶A. Messiah, *Quantum Mechanics*, Vol. 2, Wiley, N.Y., 1961 [Russ. transl. of French original, Nauka, M., 1979].
- ⁷G. Breit, Proc. Natl. Acad. Sci. U.S.A. 14, 535 (1928).
- ⁸W. Pauli, Papers on quantum mechanics (Russ. transl.), Nauka, M., 1975.
- ⁹E. Schrodinger, Sitzungsber. Dtsch. Akad. Wiss. Berlin, Kl. Math. Phys. Tech., 418 (1930).

- ¹⁰S. V. Vonsovskiĭ and M. S. Svirskiĭ in *Problems of Theoretical Physics*. Collection of articles dedicated to the memory of I. E. Tamm (In Russian) Nauka, M., 1972, p. 389.
- ¹¹S. V. Vonsovskii, M. S. Svirskii, and L. M. Svirskaya, Teor. Mat. Fiz. 85, 211 (1990) [Theor. Math. Phys. (USSR) 85, 1189 (1990)].
- ¹²S. V. Vonsovskii, M. S. Svirskii, and L. M. Svirskaya, Teor. Mat. Fiz. (1992) [Theor. Math. Phys. (USSR) (1992)].
- ¹³F. Cannata, L. Ferrari, and G. Russo, Solid State Commun. 74, 309 (1990).
- ¹⁴L. Ferrari and G. Russo, Phys. Rev. **B42**, 7454 (1990).
- ¹⁵F. Cannata and L. Ferrari, Phys. Rev. B44, 8599 (1991).

Translated by G. Volkoff