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The reflection of electrons by a potential jump according to Dirac's relativistic dynamics

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The reflection of electrons by a potential jump will be investigated using the new dynamics of Dirac. For very large values of the potential jump, as a result of the theory, electrons will push forward against the electric force that acts upon them through the jump surface and come out on the other side with a negative kinetic energy. This can be regarded as an especially striking example of the problem with relativistic dynamics that was suggested by Dirac.

Introduction. As **Dirac** (*) has emphasized, a grave dilemma exists in relativistic quantum theory in the fact that, according to that theory, an electron in a force field can take on negative energy values that are coupled with the physically-meaningful positive energy values by transition probabilities. He did not succeed in overcoming this difficulty in his new – in other respects, so successful – treatment of relativistic quantum dynamics. In the following discussion, an elementary example shall be presented in which this difficulty comes into the foreground abruptly. We shall treat the reflection and refraction of electron waves from a boundary surface where the electrostatic potential has a jump.

§ 1. Let E be the total energy of an electron that moves in a force-free region of space, while p_1, p_2, p_3 might give the components of its quantity of motion along the axes of a rectangular coordinate system in which the electron has coordinates x_1, x_2, x_3 . We would like to assume that the electrostatic potential is non-zero in that region of space, and indeed, the electron shall possess the constant potential energy P. (Naturally, this convention is meaningful only when we compare this region of space with another region of space in which the potential has a different value.) Now, from the usual relativistic mechanics, the following relation will exist between the energy $E - P$, which we would like to call the *kinetic energy* of the electron (even though it is not zero for an electron at rest, but $m_0 c^2$), and the quantity of motion:

$$\left(\frac{E-P}{c}\right)^2 = p_1^2 + p_2^2 + p_3^2 + m_0^2 c^2 , \tag{1}$$

(*) P. A. M. Dirac, Proc. Roy. Soc. **117** (1928), 612.

where m_0 means the rest mass of the electron, and c is the velocity of light. The difficulty in question is then connected with the fact that the kinetic energy can assume negative, as well as positive, values, so extra solutions with negative kinetic energies that cannot be assigned a physical meaning will be present, in addition to the physically-sensible solutions. No such difficulty exists in ordinary relativistic mechanics, due to the fact that the square of the quantity of motion can never be negative, so, from (1), the kinetic energy will never be zero. Since only continuous transitions can occur in that theory, that would mean that the negative-energy values would never be attained. However, in quantum theory, the solutions in question cannot generally be separated from each other, since, on the one hand, discontinuous radiative transitions are possible, and on the other hand, the electron waves can tunnel through regions in which the electron would have an imaginary quantity of motion, classically speaking.

§ 2. For an electron in an electrostatic force field whose potential is V, according to **Dirac**, we can associate the quantum-dynamical problem with the following wave equation:

$$\left\{\frac{E+eV}{c}+\beta mc\right\}\psi - ih\sum_{k=1}^{3}\alpha_k\frac{\partial\psi}{\partial x_k} = 0 \tag{2}$$

and its adjoint equation:

$$\varphi\left\{\frac{E+eV}{c}+\beta mc\right\} + ih\sum_{k=1}^{3}\frac{\partial\varphi}{\partial x_k}\alpha_k = 0, \tag{2a}$$

in which E again means the total energy of the electron, which we can consider to be given, while $-e$ denotes its charge, and h means Planck's constant, divided by 2π. The quantities α_1, α_2, α_3, and β are matrices with four rows and columns that satisfy the relations:

$$\left.\begin{array}{c}\alpha_i\alpha_k+\alpha_k\alpha_i=0, \quad i\neq j, \quad \alpha_i\beta+\beta\alpha_i=0, \\ \alpha_1^2=\alpha_2^2=\alpha_3^2=\beta^2=1.\end{array}\right\} \tag{3}$$

Correspondingly, the functions φ and ψ consist of four components φ_1, φ_2, φ_3, φ_4 (ψ_1, ψ_2, ψ_3, ψ_4, resp.). If γ denotes a matrix with four rows and columns then $\gamma\psi$ shall then be an abbreviation for the four quantities $\sum_{h=1}^{4}\gamma_{ik}\psi_k$ (i = 1, 2, 3, 4), in which γ_{ik} denote the matrix elements of γ; likewise, $\varphi\gamma$ shall be regarded as $\sum_{h=1}^{4}\varphi_k\gamma_{ki}$ (i = 1, 2, 3, 4). One sees that it is therefore permissible to multiply equation (2) by any matrix on the left and equation (2a) on the right without compromising their validity. That would only imply a linear transformation of the system of equations.

We would now like to assume that the potential V is equal to 0 to the left of the plane $x_1 = 0$, while one will have $eV = -P$, in which P is a positive quantity, to the right of that plane. One would then expect that under the transition through that plane, the electron would lose a part P of its kinetic energy. In order to be able to investigate the reflection and refraction of electron waves by that discontinuity surface, it will be necessary to explore the boundary conditions for discontinuity surfaces for the **Dirac** wave equations. As usual (*), one can derive it by considering the discontinuity surface to be a limiting case of a region of finite density in which the discontinuous quantity (in this case, the potential) varies rapidly. Since equations (2) can be solved for the differential quotients of the components of ψ that are perpendicular to the discontinuity surface (which are $\frac{\partial \psi_1}{\partial x_1}, \frac{\partial \psi_2}{\partial x_1}, \frac{\partial \psi_3}{\partial x_1}, \frac{\partial \psi_4}{\partial x_1}$, in this case), it will follow immediately that the potential in the transition region remains finite in such a way that the four quantities ψ_1, ψ_2, ψ_3, ψ_4 (and naturally, φ_1, φ_2, φ_3, φ_4 , as well) will remain continuous upon passing through the discontinuity surface (**).

§ 3. With no essential restriction, we can now consider a pure-harmonic incident wave that arrives perpendicular to the plane $x_1 = 0$. We then set:

$$\psi_e = v_e \, e^{\frac{i}{h}(px - Et)}, \tag{4}$$

in which we write simply x for x_1, t denotes time, and p denotes the impulse of the electron. By substituting this expression in (2), we will get a system of linear, algebraic equations for the four components of the amplitude v_e that can be written as follows:

$$\{E / c + \alpha p + \beta m_0 c\} \, v_e = 0, \tag{5}$$

in which we have replaced α_1 with α. If v_e is not supposed to vanish then that will imply the relation:

$$E^2 / c^2 = p^2 + m_0^2 c^2, \tag{6}$$

which is a special case of (1); we would then like to choose the positive value for E. Now, one is free to choose two of the components of v_e, which corresponds to just the possibility of orienting the electron in a magnetic field (***).

It follows from (6) that the impulse of the reflected wave must be $-p$, while an impulse value of $\bar{p}$ would follow for the refracted wave that would be given by the relation:

(*) Cf., H. Faxén and J. Holtsmark, Zeit. Phys. **45** (1927), 311, where a similar line of reasoning was pursued for **Schrödinger's** wave equation.

(**) Due to the solubility of equation (2) with respect to the differential quotients of the four components of ψ along an arbitrary spatial direction, it will also follow that not all four components of a continuous solution can be zero in a surface without all of them vanishing everywhere. The boundary condition $\psi = 0$ on a wall that was employed for the **Schrödinger** equation will then be meaningless in **Dirac's** theory, and must be replaced by conditions that one might learn from a closer specification of the physical behavior of the wall.

(***) Cf., C. G. Darwin, Proc. Roy. Soc. **118** (1928), 654.

$$\left(\frac{E-p}{c}\right)^2 = \bar{p}^2 + m_0^2 c^2 . \tag{7}$$

First of all, we would like to assume that P is small enough that a positive value of $\bar{p}^2$ would follow from (7). We can then set:

$$\psi_r = v_r \, e^{\frac{i}{h}(-px-Et)}, \qquad \psi_g = v_g \, e^{\frac{i}{h}(\bar{p}x-Et)}, \tag{8}$$

in which ψ_r and ψ_g belong to the reflected (refracted, resp.) waves. It will follow from (2) that:

$$\left\{\frac{E}{c} - \alpha p + \beta m_0 c\right\} v_r = 0, \qquad \left\{\frac{E}{c} + \alpha \bar{p} + \beta m_0 c\right\} v_g = 0 . \tag{9}$$

The boundary condition will now read simply:

$$v_e + v_r = v_g . \tag{10}$$

If we consider the four components of the incident wave to be given then we will have eight unknowns: namely, the four components of v_r and the four components of v_g . On the basis of (9), however, only four of these will be independent, such that (10) will provide precisely the satisfactory number of equations for its calculation. We can obtain the solution of the equations for v_r easily in the following way: It follows from (5) and the first equation (9) that:

$$(E / c + \beta m_0 c)\,(v_e + v_r) = -\,\alpha p\,(v_e - v_r).$$

If follows from (9), on the basis of (10), that:

$$(E / c + \beta m_0 c)\,(v_e + v_r) = (P / c - \alpha\,\bar{p}\,)\,(v_e + v_r),$$

and thus:

$$\{P / c - \alpha (p + \bar{p}\,)\}\, v_r = -\,\{P / c + \alpha (p - \bar{p}\,)\}\, v_e .$$

By multiplying both sides of this equation by $P / c + \alpha\,(p + \bar{p}\,)$, it follows, with consideration given to the fact that $\alpha^2 = 1$, and with the help of (6) and (7), that:

$$v_r = -\,\frac{2P/c\,(E/c + \alpha p)}{P^2/c^2 - (p+\bar{p})^2}\, v_e . \tag{11}$$

In order to be able to evaluate this result physically, we must look for the corresponding solution to the adjoint wave equation (2a), so **Dirac** would then give $\varphi\,\psi\,dv = \sum_{k=1}^{4} \varphi_k \psi_k dv$ for the probability that we would find the electron in the volume element *dv*. It would then follow from that the probability that the electron passes through the surface element *df*, which is perpendicular to the *x*-axis, in the time *dt* would be $-c\ \varphi\ \alpha\ \psi$ *df ft*, where $\varphi\ \alpha\ \psi$ is an abbreviation for $\sum_{i,k=1}^{4} \varphi_i \alpha_{ik} \psi_k$ (*). Now, as **Dirac** showed, it is possible to choose α and β to be Hermitian matrices. If ψ is a solution of equation (2) then φ (= complex conjugate of ψ) will be a solution of (2a). When we choose complex-conjugate quantities for φ and ψ, we will obviously obtain real expressions for $\varphi\ \psi$ and $\varphi\ \alpha\ \psi$ for Hermitian matrices. We then set:

$$\varphi_e = u_e\ e^{-\frac{i}{h}(px-Et)}, \qquad \varphi_r = u_r\ e^{-\frac{i}{h}(-px-Et)}, \qquad \varphi_g = u_g\ e^{-\frac{i}{h}(\bar{p}x-Et)}, \tag{12}$$

where u_e, u_r, and u_g are complex-conjugate to the quantities v_e, v_r, and v_g, in the event that α and β are Hermitian. One gets from (2a) and (12) that:

$$\left.\begin{aligned} u_e\{E/c + \beta m_0 c - \alpha p\} = 0, \qquad u_r\{E/c + \beta m_0 c + \alpha p\} = 0, \\ u_g\left\{\frac{E-P}{c} + \beta m_0 c + \alpha \bar{p}\right\} = 0. \end{aligned}\right\} \tag{13}$$

We shall now derive a useful identity from (5) and (13) when we multiply (5) by $u_e\ \alpha$ on the left and the first equation (130 by $\alpha\ v_e$ on the right. Since α and β anti-commute and $\alpha^2 = 1$, we will get, by addition, that:

$$E / c\ u_e\ \alpha\ v_e + p\ u_e\ v_e = 0,$$

or

$$-c\ u_e\ \alpha\ v_e = \frac{pc^2}{E} u_e\ v_e\ . \tag{14}$$

In the particle picture, pc^2 / E means the velocity of the electron (i.e., its group velocity), such that this equation will give a connection between the current density and the density that is the same as the correspondence in ordinary hydrodynamics. Naturally, similar things are true for the reflected and the refracted waves (for the latter, E must be replaced with the kinetic energy $E - P$). For the calculation of the fractions of the electrons that are reflected (refracted, resp.), it will then suffice to express the quantities $u_r\ v_r$ and $u_g\ v_g$ in terms of the components of the incident wave.

By a calculation that is similar to the one that led to the expression (11), we will now find that:

$$u_r = -\ u_e\ \frac{2P/c\,(E/c + \alpha p)}{P^2/c^2 - (p+\bar{p})^2}\ . \tag{15}$$

It will then follow from (10) and (15) that:

(*) P. A. M. Dirac, Proc. Roy. Soc. **118** (1928), 351.

$$u_r\,v_r\left(\frac{2P/c}{P^2/c^2-(p+\bar{p})^2}\right)^2 u_e\,(E/c+\alpha p)^2\,v_e$$
$$=\left(\frac{2P/c}{P^2/c^2-(p+\bar{p})^2}\right)^2\left\{(E^2/c^2+p^2)u_e v_e+\frac{2Ep}{c}u_e\alpha v_e\right\},$$

or, from (14) and (6):

$$u_r\,v_r=\left(\frac{2P/c}{P^2/c^2-(p+\bar{p})^2}\right)^2 u_e\,v_e\,. \tag{16}$$

The quantity $\left(\frac{2P/c}{P^2/c^2-(p+\bar{p})^2}\right)^2$ will then give the fraction of the electrons that are reflected. As one easily confirms with the help of (6) and (7), this reflection coefficient increases with increasing P from zero for $P = 0$ and attains the value unity for $P = E - m_0c^2$. Now, $\bar{p}^2$ is equal to zero, here, and for a further increase of P, we will enter into the domain of imaginary $\bar{p}$, which we would now like to investigate.

In the classical theory, the notion of $\bar{p}$ becoming imaginary would mean that the electron goes so far into the field that its velocity becomes zero and is then pushed back out. In wave theory, the wave functions will also have finite values on the right of the boundary surface, as we have seen, which will correspond to the phenomenon of total reflection in optics.

If $\bar{p}$ is imaginary then we can set:

$$\psi_g=v_g\;e^{-\mu x-iEt/h},\qquad \gamma_g=u_g\;e^{-\mu x+iEt/h}, \tag{17}$$

in which μ means a real quantity that must obviously be positive, since otherwise the density on the right of the boundary surface would increase to infinity with x. It is just because μ is real in this case that, from the general prescriptions of the theory, the exponents in ψ_g and φ_g that are proportional to x must have the same signs. However, that would mean that we would set the quantity $\bar{p}$ equal to $ih\mu$ for ψ_g, but equal to $-ih\mu$ for φ_g. With that convention, we will get from (11) and (15) that:

$$v_r=-\frac{2P/c\,(E/c+\alpha p)}{P^2/c^2-(p+ih\mu)^2}\;v_e\,,\qquad u_r=-\,u_e\,\frac{2P/c\,(E/c+\alpha p)}{P^2/c^2-(p-ih\mu)^2}\,, \tag{18}$$

and then:

$$u_r\,v_r=\frac{(2P/c)^2\,(E^2/c^2-p^2)}{[(P/c+p)^2+\mu^2h^2][(P/c-p)^2+\mu^2h^2]}\;u_e\,v_e\,.$$

We can simplify this expression with the help of (6) and (7). It will then follow that:

$$\bar{p}^2 = p^2 - \frac{P(2E - P)}{c^2}, \tag{19}$$

and thus, with $\bar{p}^2 = -\mu^2 h^2$:

$$(P / c \pm p)^2 + \mu^2 h^2 = 2\, P / c\, (E / c \pm p).$$

For that reason, it will follow simply that:

$$u_r\, v_r = u_e\, v_e\,. \tag{20}$$

The reflected current will then be equal to the incident current, while an exponentially-decreasing wave solution will exist behind the boundary surface. From (19), the condition for this case is $p^2 < \frac{P(2E - P)}{c^2}$, which is a condition that will be first fulfilled for increasing P when P exceeds the value of $E - c\sqrt{E^2 / c^2 - p^2} = E - m_0\, c^2$. If P increases further then the quantity μ will first increase; however, due to the quadratic terms in P in (19), it will attain a maximum that happens when $P = E$. From there on, μ will become smaller, and it will again become zero for $P = E + c\sqrt{E^2 / c^2 - p^2} = E + m_0\, c^2$. For still larger P, $\bar{p}$ will assume real values, such that formulas (11), (15), and (16) will once more represent the solution to the problem. As a result, the kinetic energy $E - P$ will be negative in that domain, such that we have actually arrived in the mechanically-forbidden domain. This has the consequence that the group velocity, which is given by $\frac{c^2}{E - P}\,\bar{p}$, is directed opposite to the impulse, and we must take a negative value for $\bar{p}$ (*). One sees this easily when one chooses the initial state to be a wave group that moves from the left to the boundary surface.

We have then arrived at the peculiar result that for values of P that are larger than $E + m_0\, c^2$, a fraction of the electrons will pass through the potential jump, while their kinetic energy will be converted from the original positive value to a negative value. It is interesting to calculate the group velocity of these electrons that pass through. In order for that to be true, it will follow from (7) that:

$$\frac{c^2}{P - E}\,|\,\bar{p}\,| = c\,\sqrt{1 - \left(\frac{m_0 c^2}{P - E}\right)^2}\,. \tag{21}$$

For $P = E + m_0\, c^2$, this velocity is, as one would expect, equal to zero precisely. It will then increase with increasing P until it attains the velocity of light for $P = \infty$.

(*) I originally did not notice this situation, but it was pointed out to me in a conversation with W. Pauli, to whom I am deeply grateful.

The reflection coefficient, which is equal to unity for $P = E + m_0 c^2$, will, as one sees from the expression (16), decrease gradually to the value $\frac{E/c - p}{E/c + p}$ for $P = \infty$. The corresponding boundary value for the fraction of the electrons that pass through the boundary surface will then be $\frac{2p}{E/c + p}$; i.e., it will be of the same order of magnitude as the ratio of the velocity of the incident electrons to the velocity of light, and can assume considerable values for large values of p. For $p = m_0 c$ that corresponds to a velocity of the incident electrons of (say) 70% of the velocity of light, we will get – e.g. – the value $2(\sqrt{2} - 1)$; i.e., perhaps 83%. Naturally, it is not essential that we have chosen $P = \infty$ here; obviously, one would get numbers of the same order of magnitude, as long as P is several times larger than the rest energy $m_0 c^2$ of the electron. We would not like to go into the question here of the possibility that such potential jumps can be realized experimentally. We shall only emphasize that the difficulty in question is not linked to the assumption of discontinuity, which was chosen only in order to simplify the mathematics. Even when the jump surface is replaced with a small region in which the potential increases rapidly, according to the theory, and as would emerge from the manner of calculation, electrons will pass into the forbidden domain where they possess negative kinetic energies, which is closely connected to the fact that in the case of total reflection that was discussed above, the wave solution did not vanish behind the boundary surface, even though the electron would possess an imaginary quantity of motion there according to classical mechanics. Let it also be mentioned that as a result of the reflection coefficient of electrons that pass from a region of space in which the potential energy is P through the boundary surface and into free space, the expression (16) will have the same values as the reflection coefficient for the opposite process.

As the result of what we did, we can then assert that the difficulty that **Dirac** pointed out in relativistic quantum mechanics can appear under circumstances that already happen for purely mechanical problems in which one does not speak of any radiative processes.

At the conclusion of this note, I would like to extend my deepest thanks to Herrn Professor N. Bohr for many conversations that contributed essentially to the clarification of the arguments above.

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