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Nonrelativistic approximations of the relativistic equations and subbarrier relativistic effects

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Abstract. It is proved that subbarrier relativistic effects, which are due to the magnitude of quasi-momentum, give a significant contribution to the penetration coefficient. For instance, an account of these effects for penetration of low-energy π^+ mesons through the Coulomb barrier of the ^{238}U nucleus would increase the penetration coefficient by 20% compared with the nonrelativistic value. We suggest to calculate the tunnelling ability by the use of a quasi-relativistic Schrödinger equation which we obtain as a reduction of the Dirac or Klein–Gordon equation, and it coincides with the reduced Bethe–Salpeter equation. Standard nonrelativistic expressions for the current and boundary conditions are revised.

1. Introduction

The tunnelling problem has been the subject of intensive investigations since the time quantum mechanics arose, due to its various applications ranging from quantum field theory (vacuum–vacuum tunnelling) to technical problems (tunnelling in diodes). The standard textbook way of describing this phenomenon is through the solution of the nonrelativistic Schrödinger equation (in the presence of the relevant potential) followed by a calculation of the penetration ability. The use of the *nonrelativistic* equation comes from the assumption that the *nonrelativistic* approximation of energy conservation is valid,

$$\sqrt{m^2+\boldsymbol{k}^2}+V(r)=E_{\rm kin}^0+m \qquad \Rightarrow \qquad \frac{\boldsymbol{k}^2}{2m}+V(r)=E_{\rm kin}^0 \tag{1}$$

where $E_{\rm kin}^0$ is the initial kinetic energy, $V(r)$ is the potential energy, m is the particle mass, and the system of units $\hbar=c=1$ is adopted. It is a satisfactory approach to the problem outside the barrier region where $V(r)\leqslant E_{\rm kin}^0\ll m$. However, it is not satisfactory for a range of magnitudes of $V(r)$ and $E_{\rm kin}^0$ in the subbarrier region. Indeed, in the subbarrier region the momentum becomes imaginary $k=\mathrm{i}q$, where $q=[2m(V(r)-E_{\rm kin}^0)]^{1/2}$ is the so-called quasi-momentum. Then the validity of approximation (1) can change drastically for a strong enough potential ($V(r)\to m$) and small initial kinetic energy ($E_{\rm kin}^0\to 0$) when the quasi-momentum becomes comparable with the particle mass, m. This means that the energy balance might be controlled by (for instance, for the Coulomb potential in the region where $r\to 0$)

$$\sqrt{m^2-q^2}+V(r)=E_{\rm kin}^0+m. \tag{2}$$

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Nevertheless we investigate a particle which moves very slowly in the 'free' domain (i.e. where $V(r) = 0$). A small initial energy guarantees the absence of the Klein paradox [1], and therefore pair creation along the penetration path is of no significance. Of course, the latter statement is not valid for the region with $V(r) \geqslant 2m + E^0_{\mathrm{kin}}$ (the region of the Klein paradox) where a single-particle description is no more applicable.

In the present paper we deal with a specific relativistic phenomenon which arises due to large values of the quasi-momentum in the subbarrier domain and small values of the free momentum k_{in}, where $k^2_{\mathrm{in}}/2m = E^0_{\mathrm{kin}}$ far from the barrier. To investigate this regime we would like to have a relativistic equation providing a reliable probabilistic treatment for spinless particles [2].

A suitable equation can be obtained by splitting the Dirac equation into positive-energy and negative-energy subspaces or by a reduction of the Klein–Gordon equation to positive-energy states [3]. Both approaches are valid for the limited kinematic region $E_{\mathrm{kin}} \leqslant m$. In the presence of an external scalar field V, which could be regarded also as a zero component of a four-vector, the equation reads

$$\mathrm{i}\hbar \frac{\partial \psi(t, \boldsymbol{r})}{\partial t} = (H_0 + V)\psi(t, \boldsymbol{r}) \tag{3}$$

where

$$H_0 = \sqrt{m^2 + \hat{\boldsymbol{k}}^2} \tag{4}$$

with $\hat{k}_j = -\mathrm{i}\hbar\partial/\partial x_j$ and $j = 1, 2, 3$. At the same time equation (3) is an approximation to the Bethe–Salpeter equation for spinless particles when the kernel is evaluated for the instantaneous interaction. It has been widely used in studying the quarkonium problem [4].

For further applications it should be mentioned that the eigenfunctions of the free particle operator H_0 are the plane waves $\psi(\boldsymbol{r}) = c(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$, with eigenvalues $E = \sqrt{m^2 + \boldsymbol{k}^2}$, and also exponentially increasing and decreasing functions $\psi(\boldsymbol{r}) = c(\boldsymbol{q})\mathrm{e}^{\boldsymbol{q}\cdot\boldsymbol{r}}$, with eigenvalues $E = \sqrt{m^2 - \boldsymbol{q}^2}$ ($|\boldsymbol{q}| \leqslant m$). As shown in [5], the set of such solutions for positive energies forms a linear space which can be transformed into a Hilbert space. The features of the non-local operator H_0 are discussed in more detail in [6].

In momentum representation the action of the operator $H_0(\boldsymbol{r})$ on the wavefunction is

$$H_0\psi(t, \boldsymbol{r}) = \frac{1}{(2\pi)^3} \int \mathrm{d}^3k\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{r}} \sqrt{m^2 + \boldsymbol{k}^2}\, \psi(t, \boldsymbol{k}). \tag{5}$$

This Hamiltonian has been exploited with various potentials to describe two-particle [7] and many-particle bound states [8].

The paper is organized in the following way. Starting from the Dirac equation we obtain in section 2.1 equation (3) for the energy sector $E^0_{\mathrm{kin}} + V \leqslant 2m$. The nonrelativistic approximations to the Klein–Gordon equation are discussed in section 2.2. Based on equation (3) in section 3.1 we revise the standard expressions for the current and the boundary conditions. In section 3.2 we apply these results to investigate the penetration of a particle to a barrier of constant height. Section 3.3 is devoted to an investigation of the penetration of positively charged particles to the Coulomb barrier of a heavy nucleus. Finally in section 4, the results are discussed and summarized.

2. Nonrelativistic approximations of the relativistic equations

2.1. Splitting of the Dirac equation

In this section we obtain the quasi-relativistic Schrödinger-like equation as a result of step-by-step operations:

(1) reduction of the bispinor Dirac equation to the spinor form;

(2) factorization of the spinor Dirac operator into a product where one factor corresponds to the positive energy states and the other one to negative energy states;

(3) to project to positive energy states we consider a special kind of external field $A = \{A_0(t), \boldsymbol{A}(\boldsymbol{r})\}$ so that all relativistic corrections can be represented in a condensed form.

There are two basic methods used to obtain the nonrelativistic approximations of the Dirac equation: the Pauli elimination method [9, 10] and the Foldy–Wouthuysen unitary transformation method [11]. It should be mentioned that the Pauli elimination method [9] has been troubled by some nonhermiticity problems, but they have been overcome by Akhiezer and Berestetsky [10] for the second-order corrections ($\propto 1/c^2$). In the present paper we explore the extended or generalized elimination scheme applied to the Dirac [12] and Klein–Gordon equation as well. This formalism makes it possible to take into account all dynamic relativistic corrections [3].

The Dirac equation for a spin-$\frac{1}{2}$ particle in an external electromagnetic field

$$\{A_0(t, \boldsymbol{r}), \boldsymbol{A}(t, \boldsymbol{r})\}$$

reads

$$\left[\mathrm{i}\frac{\partial}{\partial t} - \mathrm{e}A_0\right]\Psi = [\boldsymbol{\alpha}\cdot(\hat{\boldsymbol{p}} - \mathrm{e}\boldsymbol{A}) + \beta m]\Psi \tag{6}$$

where

$$\hat{\boldsymbol{p}} = -\mathrm{i}\boldsymbol{\nabla} \qquad \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

the σ_i $(i = 1, 2, 3)$ are the Pauli matrices and I is the 2×2 unit matrix.

Let us introduce the dimensionless energy and momentum-type operators

$$\hat{\epsilon} = \frac{1}{2m}\left(\mathrm{i}\frac{\partial}{\partial t} - \mathrm{e}A_0\right) \tag{7}$$

$$\hat{\pi}_\sigma = \frac{1}{2m}\boldsymbol{\sigma}\cdot(\hat{\boldsymbol{p}} - \mathrm{e}\boldsymbol{A}). \tag{8}$$

We now go over from the initial bispinor Ψ to slowly varying spinors $\phi(t, \boldsymbol{r})$ and $\chi(t, \boldsymbol{r})$ by means of the unitary transformation

$$\Psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \exp(-\mathrm{i}mt) \tag{9}$$

which means that from now on we investigate the positive energy states. It is clear that after this transformation the operator $\mathrm{i}\partial/\partial t$ applied to spinor ϕ becomes the operator of the kinetic energy $E_{\mathrm{kin}} = E - m$ (E is the total energy) and the operators defined through equations (7) and (8) after the action on the upper spinor have the following orders of magnitude:

$$\hat{\epsilon}\phi \approx \frac{E_{\mathrm{kin}} - \mathrm{e}A_0}{2m}\phi \approx \frac{1}{c^2}\phi \tag{10}$$

$$\hat{\pi}_\sigma\phi \approx \frac{|\boldsymbol{p} - \mathrm{e}\boldsymbol{A}|}{2m}\phi \approx \frac{1}{c}\phi. \tag{11}$$

Using definitions (7) and (8), the Dirac equation (6) is written as a system of coupled equations for spinors ϕ and χ

$$\hat{\epsilon}\phi = \hat{\pi}_\sigma \chi \tag{12}$$

$$(I + \hat{\epsilon})\chi = \hat{\pi}_\sigma \phi. \tag{13}$$

The solution of equation (13) may be expressed in the following symbolic form

$$\chi = (I + \hat{\epsilon})^{-1}\hat{\pi}_\sigma \phi \tag{14}$$

where the function of the operator here and below is defined by the series corresponding to this function. As will be seen, satisfying the conditions $E_{\mathrm{kin}} - \mathrm{e}A_0 < 2m$ and $|\boldsymbol{p} - \mathrm{e}\boldsymbol{A}| < 2m$ is quite enough for convergence of the Taylor series in operators $\hat{\epsilon}$, $\hat{\pi}_\sigma$ and their combinations. On the other hand, one can regard all functions of the operators under consideration here in the spirit of the nonrelativistic approximation and then truncate the series for the required order of approximation. In this case the convergence of the series is out of the question.

The problem of the existence of an inverse operator appears throughout further considerations, and we state the following lemma.

Lemma. A positive-definite operator always has an inverse one.

In particular, if the differential equation in operator form reads

$$\hat{B}\hat{A}\phi(\boldsymbol{r}, t) = 0 \tag{15}$$

and $\hat{B}$ is a positive-definite operator (no negative and zero eigenvalues, or/and the equation $\hat{B}\phi = b\phi$ implies that $b > 0$), then the reduced equation

$$\hat{A}\phi(\boldsymbol{r}, t) = 0 \tag{16}$$

is valid.

An intuitive proof of this reduction may be carried out if we employ an iteration procedure to the equation $(I - \hat{\delta})\hat{A}\phi = 0$, where $\hat{\delta}$ is small in comparison with I. In the iteration we obtain the sequence

$$\hat{A}\phi = \hat{\delta}\hat{A}\phi \qquad \hat{A}\phi = \hat{\delta}^2\hat{A}\phi \ldots \hat{A}\phi = \hat{\delta}^n\hat{A}\phi \qquad \Rightarrow \quad \hat{A}\phi = 0 \tag{17}$$

which leads to equation (16). Having excluded the 'small' spinor χ from equations (12) and (13), we obtain

$$\hat{\epsilon}\phi = \hat{\pi}_\sigma(I + \hat{\epsilon})^{-1}\hat{\pi}_\sigma\phi. \tag{18}$$

Equation (18) is relative to the upper spinor ϕ and should not be regarded as the Schrödinger equation since the spinor ϕ is not normalized to unity. Indeed, it follows from the normalization of the initial bispinor that

$$\int [\phi^+\phi + \phi^+\hat{\pi}_\sigma(I + \hat{\epsilon})^{-2}\hat{\pi}_\sigma\phi]\,\mathrm{d}^3r = 1. \tag{19}$$

Taking this as a guide [10] it is reasonable to go over to a new normalized spinor

$$f(\boldsymbol{r}, t) = [I + \hat{\pi}_\sigma(I + \hat{\epsilon})^{-2}\hat{\pi}_\sigma]^{1/2}\phi(\boldsymbol{r}, t) \tag{20}$$

where the last transformation is a Hermitian one. Indeed, the momentum-type operator $\hat{\pi}_\sigma$ is Hermitian. Then, if one regards equation (18) as an iteration algorithm for evaluating the operator $\hat{\epsilon}$, taking into account, equations (10) and (11), the leading approximation is

$$\hat{\epsilon}\phi = \hat{\pi}_\sigma^2\phi. \tag{21}$$

Therefore, after a number of iteration steps the energy-type operator $\hat{\epsilon}$ is represented to any order of approximation as a sum of powers $\hat{\pi}_\sigma^2$ and thus is Hermitian with respect to the state space of spinors ϕ. So, the Hermitian transformation (20) gives us a new spinor f which is rigorously normalized to unity

$$\int f^+ f \, \mathrm{d}^3 r = 1. \tag{22}$$

Having expressed ϕ via f and substituted it into equation (18), we obtain a new equation for the spinor f,

$$\hat{\epsilon}[I + \hat{\pi}_\sigma (I + \hat{\epsilon})^{-2} \hat{\pi}_\sigma]^{-1/2} f(\boldsymbol{r}, t) = \hat{\pi}_\sigma (I + \hat{\epsilon})^{-1} \hat{\pi}_\sigma [I + \hat{\pi}_\sigma (I + \hat{\epsilon})^{-2} \hat{\pi}_\sigma]^{-1/2} f(\boldsymbol{r}, t). \tag{23}$$

Equation (23) has been obtained to an arbitrary order of approximation (or formally even without any approximation). Thus, the bispinor Dirac equation (6) was transformed in a condensed form to the spinor equation (23). It is quite reasonable to look for nonrelativistic spinor approximations to the Dirac equation on the basis of equation (23).

Let us study the structure of equation (23). For this purpose we assume the special case of an external field

$$A = (A_0(t), \boldsymbol{A}(\boldsymbol{r})) \tag{24}$$

more formally it means

$$[\hat{\epsilon}, \hat{\pi}_\sigma] = 0. \tag{25}$$

Using this condition, one can make further transformations on equation (23). We consider equation (23) in view of the above lemma regarding $\hat{B}$ as the operator

$$\hat{B} \equiv [I + \hat{\pi}_\sigma (I + \hat{\epsilon})^{-2} \hat{\pi}_\sigma]^{-1/2} \equiv I + \hat{\delta}. \tag{26}$$

In fact, the definition of $\hat{\delta}$ in this equation implies the series

$$\hat{\delta} = (I + \hat{\epsilon})^{-2} [-\tfrac{1}{2} \hat{\pi}_\sigma^2 + \tfrac{3}{8} \hat{\pi}_\sigma^4 - \tfrac{15}{48} \hat{\pi}_\sigma^6 + \ldots] \propto \tfrac{1}{c^2} + \mathrm{O}(\tfrac{1}{c^2}) \tag{27}$$

and thus the operator $(I + \hat{\delta})$ is indeed positive-definite.

With the commutator (25) and the above definition of $\hat{B}$, equation (23) reduces to

$$\hat{\epsilon}(I + \hat{\epsilon}) f(\boldsymbol{r}, t) = \hat{\pi}_\sigma^2 f(\boldsymbol{r}, t). \tag{28}$$

It should be pointed out that in the process of deriving the last equation we use the commutation of the operator $\hat{B}$ (defined by equation (26)) with the first three factors on the right-hand side of equation (23). However, in the general case, when equation (25) is absent, commuting $\hat{B}$ to the left yields new terms proportional to the derivatives of the external field.

At the next level of transformations one can represent equation (28) with respect to the commutation relation (25) in the form

$$[\hat{\epsilon} - \epsilon_-(\hat{\pi}_\sigma^2)][\hat{\epsilon} - \epsilon_+(\hat{\pi}_\sigma^2)] f(\boldsymbol{r}, t) = 0 \tag{29}$$

where $\epsilon_-(x)$ and $\epsilon_+(x)$ are

$$\epsilon_-(\hat{\pi}_\sigma^2) = -\tfrac{1}{2}[I + \sqrt{I + 4\hat{\pi}_\sigma^2}] \tag{30}$$

$$\epsilon_+(\hat{\pi}_\sigma^2) = \tfrac{1}{2}[-I + \sqrt{I + 4\hat{\pi}_\sigma^2}]. \tag{31}$$

The first operator function $\epsilon_-(\hat{\pi}_\sigma^2)$ corresponds to the negative energy states and the second one $\epsilon_+(\hat{\pi}_\sigma^2)$ to the positive energy states. Thus, for the special kind of external field (5), there is a possibility to factorize (or to split) the spinor Dirac operator in an explicit manner to factors which determine the positive and negative energy states.

Meanwhile, it is evident that the negative energy operator (the first bracket in equation (29)) is positive-definite and has the structure $(I + \hat{\delta})$. Indeed, we have

$$\hat{\epsilon} - \epsilon_- \left(\hat{\pi}_\sigma^2\right) \approx I + \hat{\epsilon} + \hat{\pi}_\sigma^2 + \mathrm{O}\left(\frac{1}{c^2}\right). \tag{32}$$

Thus, according to the lemma, equation (29) can be reduced to

$$[\hat{\epsilon} - \epsilon_+(\hat{\pi}_\sigma^2)] f(\boldsymbol{r}, t) = 0 \tag{33}$$

or

$$\hat{\epsilon} f(\boldsymbol{r}, t) = \tfrac{1}{2}[\sqrt{I + 4\hat{\pi}_\sigma^2} - I] f(\boldsymbol{r}, t). \tag{34}$$

So we obtain a Dirac spinor equation for the particles with positive energy ($\epsilon_+(x) > 0$). In the generally accepted notation equation (34) appears as

$$\mathrm{i}\frac{\partial \psi}{\partial t} = (H_D^{(1)}(\boldsymbol{r}) + V(t))\psi \tag{35}$$

with the Hamiltonian

$$H_D^{(1)}(\boldsymbol{r}) = \sqrt{m^2 + (-\mathrm{i}\boldsymbol{\nabla} - \mathrm{e}\boldsymbol{A}(\boldsymbol{r}))^2 - \mathrm{e}\boldsymbol{\sigma} \cdot \boldsymbol{B}(\boldsymbol{r})} \qquad V(t) = \mathrm{e}A_0(t) \tag{36}$$

where $\boldsymbol{B} = \nabla \times \boldsymbol{A}$. We have made reverse unitary transformation of the wavefunction

$$\psi = f \;\; \exp(-\mathrm{i}mt) \tag{37}$$

from which, with to equation (22), follows that

$$\int \psi^+ \psi \, \mathrm{d}^3 r = 1. \tag{38}$$

Under the square root in equation (36) one can recognize the Hamiltonian of the Pauli equation. On the other hand, the Pauli equation can be obtained if we preserve the first term only in the series corresponding to this root. The next two terms of this series coincide with the well known second and fourth order relativistic corrections.

Equations (35) and (36) may be regarded as a rigorous Dirac spinor equation for energy- and momentum-type operators that satisfy the inequality

$$\| \hat{\epsilon} \| < 1 \qquad \| \hat{\pi}_\sigma^2 \| < 1 \tag{39}$$

which is quite enough for convergence of the above series. For weak fields it means that the particle energy sector is restricted to $0 < E < 2m$, where $E = (m^2 + p^2)^{1/2}$.

In the case of an arbitrary external electromagnetic field, the new terms, which are proportional to the derivatives of the field, appear in addition to the Hamiltonian (36). These new terms are the commutation products which are due to transferring the wavefunction normalization factor (square brackets in equation (23)) to the left position, with the aim of extracting it as a positive-definite operator (see the lemma). Then, in the explicit form they appear as an expansion in powers of $1/c$. For example, the Hamiltonian, which includes the second order field corrections, reads as

$$H^{(2)} = H_D^{(1)}(t, \boldsymbol{r}) + \mathrm{e}A_0(t, \boldsymbol{r}) - \frac{\mathrm{e}}{8m^2}\{\nabla \cdot \boldsymbol{E} + \mathrm{i}\boldsymbol{\sigma} \cdot (\nabla \times \boldsymbol{E}) + 2\boldsymbol{\sigma} \cdot [\boldsymbol{E} \times (-\mathrm{i}\boldsymbol{\nabla} - \mathrm{e}\boldsymbol{A})]\} \tag{40}$$

where $\boldsymbol{E} = -\boldsymbol{\nabla} A_0 - \partial \boldsymbol{A}/\partial t$.

The higher-order corrections yield higher-order derivatives of the external field. When dealing with nonrelativistic approximations in the case of a smooth external field, it is enough in practice to take into account the third- or fourth-order field derivatives.

It should be pointed out that the use of the Hamiltonian

$$H_D^{\rm nonrel}(t,\boldsymbol{r}) = \sqrt{m^2 + (-{\rm i}\boldsymbol{\nabla} - {\rm e}\boldsymbol{A}(t,\boldsymbol{r}))^2 - {\rm e}\boldsymbol{\sigma}\cdot\boldsymbol{B}(t,\boldsymbol{r})} + V(t,\boldsymbol{r}) \qquad (41)$$

implies that the potential $V(t,\boldsymbol{r})$ can be regarded firstly in a sense of the nonrelativistic approximation (see equation (40)). Then, it equals ${\rm e}A_0(t,\boldsymbol{r})$ plus a truncated series of the field derivatives (expansion in powers of $1/c$) where all terms can be calculated in principle to any fixed order. On the other hand, $V(t,\boldsymbol{r})$ can be taken as an effective or phenomenological potential in place of the nonrelativistic approximation.

2.2. Reduction of the Klein–Gordon equation

The same scheme may be applied to the Klein–Gordon equation describing a scalar particle in the external electromagnetic field $\{A_0(t,\boldsymbol{r}), \boldsymbol{A}(t,\boldsymbol{r})\}$

$$\left({\rm i}\frac{\partial}{\partial t} - {\rm e}A_0\right)^2 \Psi = [(\hat{\boldsymbol{p}} - {\rm e}\boldsymbol{A})^2 + m^2]\Psi. \qquad (42)$$

We introduce the dimensionless energy and momentum-type operators

$$\hat{\epsilon} = \frac{1}{2m}\left({\rm i}\frac{\partial}{\partial t} - {\rm e}A_0\right) \qquad (43)$$

$$\hat{\pi}_i = \frac{1}{2m}(\hat{p}_i - {\rm e}A_i). \qquad (44)$$

After transforming the wavefunction to the ‘slow’ one

$$\Psi = \phi {\rm e}^{-{\rm i}mt} \qquad (45)$$

we arrive at the equation

$$\hat{\epsilon}(I + \hat{\epsilon})\phi(\boldsymbol{r},t) = \hat{\pi}^2\phi(\boldsymbol{r},t) \qquad (46)$$

which has the same structure as equation (28). Overcoming the problem of normalization of the wavefunction in the same manner as in the spin-particle case for a particular external field $A = (A_0(t), \boldsymbol{A}(\boldsymbol{r}))$, we factorize equation (46) as

$$[\hat{\epsilon} - \epsilon_-(\hat{\pi}^2)][\hat{\epsilon} - \epsilon_+(\hat{\pi}^2)]\phi(\boldsymbol{r},t) = 0 \qquad (47)$$

where $\epsilon_-(x)$ and $\epsilon_+(x)$ are

$$\epsilon_-(\hat{\pi}^2) = -\tfrac{1}{2}[I + \sqrt{I + 4\hat{\pi}^2}] \qquad (48)$$

$$\epsilon_+(\hat{\pi}^2) = \tfrac{1}{2}[-I + \sqrt{I + 4\hat{\pi}^2}]. \qquad (49)$$

Obviously, the first operator factor in equation (47) (or the Hamiltonian (48)) corresponds to the negative energy states, whereas the second operator factor (or the Hamiltonian (49)) corresponds to the positive energy states. It is straightforward to prove in the same manner as was done for equations (26) and (27) that the first operator factor in equation (47) is positive-definite. Therefore (see the lemma), we come to the reduced equation

$$\hat{\epsilon}\ \phi(\boldsymbol{r},t) = \epsilon_+(\hat{\pi}^2)\phi(\boldsymbol{r},t). \qquad (50)$$

In the generally accepted notation it appears as

$${\rm i}\frac{\partial\psi}{\partial t} = [\sqrt{m^2 + (-{\rm i}\boldsymbol{\nabla} - {\rm e}\boldsymbol{A}(\boldsymbol{r}))^2} + {\rm e}A_0(t)]\psi \qquad (51)$$

where we have made a transformation inverse to equation (45) on the wavefunction ϕ. The new wavefunction ψ obtained is normalized exactly to unity.

For a general external field the structure of the Hamiltonian in equation (51) is still unchanged, except that there appear new terms proportional to the derivatives of the field. In the same way as discussed at the end of the previous section, the Klein–Gordon Hamiltonian in the nonrelativistic approximation has the form

$$H_{\mathrm{KG}}^{\mathrm{nonrel}} = \sqrt{m^2 + (-\mathrm{i}\boldsymbol{\nabla} - \mathrm{e}\boldsymbol{A}(t, \boldsymbol{r}))^2} + V(t, \boldsymbol{r}) \tag{52}$$

where $V(t, \boldsymbol{r}) = \mathrm{e}A_0(t, \boldsymbol{r}) + (truncated\ series)$, or $V(t, \boldsymbol{r})$ is an effective potential which arises from a phenomenological approach.

If the vector components of the external field are absent (thus there are no spin effects), the Hamiltonian (36) degenerates to a scalar operator and coincides literally with the Hamiltonian of equation (51). In the next sections we explore this Hamiltonian in order to investigate tunnelling phenomena.

3. Subbarrier relativistic effects

3.1. Continuity equation and boundary condition

The Schrödinger equation, as well as other equations with the first derivative in time, appear attractive due to the fact that they admit of a probabilistic interpretation. Specifically, this interpretation is achieved because it is possible to construct the continuity equation

$$\frac{\partial \rho(t, \boldsymbol{r})}{\partial t} + \mathrm{div}\, \boldsymbol{j}(t, \boldsymbol{r}) = 0. \tag{53}$$

It can be derived from the Lagrangian, if any, or directly from the equation of motion. In this section we use equation (51) when $\boldsymbol{A} = 0$ and rewrite it in a somewhat generalized form regarding the term $\mathrm{e}A_0$ as an external potential V:

$$\mathrm{i}\frac{\partial \psi}{\partial t} = (\sqrt{m^2 - \boldsymbol{\nabla}^2} + V)\psi. \tag{54}$$

From a combination of this equation and its complex conjugate we obtain

$$\rho(t, \boldsymbol{r}) = \psi^*(t, \boldsymbol{r})\psi(t, \boldsymbol{r}) \tag{55}$$

i.e. the ordinary quantum-mechanical probability density, and also

$$\mathrm{div}\ \ \boldsymbol{j}(t, \boldsymbol{r}) = -\mathrm{i}(\psi H_0 \psi^* - \psi^* H_0 \psi). \tag{56}$$

The solution of this equation for the current $\boldsymbol{j}$ (see the appendix for details) can be presented as

$$j_i(t, \boldsymbol{r}) = \left[\frac{\hat{k}_i(\boldsymbol{r}) - \hat{k}_i(\boldsymbol{r}')}{H_0(\boldsymbol{r}) + H_0(\boldsymbol{r}')} \psi(t, \boldsymbol{r})\psi^*(t, \boldsymbol{r}') \right]_{\boldsymbol{r}'=\boldsymbol{r}} \tag{57}$$

where $\hat{k}_i(\boldsymbol{r}') = -\mathrm{i}\partial/\partial x'_i$ and $H_0(\boldsymbol{r}') = \sqrt{m^2 + \hat{\boldsymbol{k}}^2(\boldsymbol{r}')}$.

For the plane wave $\psi(t, \boldsymbol{r}) = \alpha \exp(-\mathrm{i}Et + \mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r})$ with the corresponding probability density $\rho = \alpha^*\alpha$, we get using equation (57),

$$\boldsymbol{j} = \frac{\boldsymbol{k}}{\sqrt{m^2 + \boldsymbol{k}^2}} \alpha^*\alpha = \boldsymbol{v}_{\mathrm{rel}}\rho. \tag{58}$$

This result agrees with the generally accepted notion that for a free-like propagation a probability flow is the probability density multiplied by the particle velocity, which now is a relativistic one.

Let us consider stationary processes and, for simplicity, take only one space dimension. In this case equation (54) is rewritten as

$$H_0\psi(x) = [E - V(x)]\psi(x) \tag{59}$$

where $H_0 = \sqrt{m^2 - \nabla^2}$ and $\psi(t, x) = \exp(-\mathrm{i}Et)\psi(x)$. To preserve a probabilistic interpretation we have to assume that the wavefunction is continuous on the boundaries of spatial regions. The boundary conditions on the derivatives can be found from equation (59). Integrating equation (59) from $(x_0 - \Delta)$ to $(x_0 + \Delta)$, we obtain

$$\int_{x_0-\Delta}^{x_0+\Delta} \left(\sqrt{\hat{k}^2 + m^2} - m\right)\psi(x)\,\mathrm{d}x = \int_{x_0-\Delta}^{x_0+\Delta} [E^0_{\mathrm{kin}} - V(x)]\psi(x)\,\mathrm{d}x \tag{60}$$

where $E^0_{\mathrm{kin}} = E - m$. Due to the continuity of $\psi(x)$ and the finiteness of the potential energy jump on the boundary x_0 of two regions, the right-hand side integral is zero in the limit $\Delta \to 0$. After an identical transformation of the integrand in the left-hand side of equation (60) we obtain

$$\int_{x_0-\Delta}^{x_0+\Delta} \frac{\hat{k}^2}{\sqrt{\hat{k}^2 + m^2} + m}\psi(x)\,\mathrm{d}x = 0. \tag{61}$$

This equation just gives the boundary conditions for the derivatives of the wavefunction

$$\frac{\hat{k}}{\sqrt{\hat{k}^2 + m^2} + m}\psi(x_0 - 0) = \frac{\hat{k}}{\sqrt{\hat{k}^2 + m^2} + m}\psi(x_0 + 0). \tag{62}$$

It is clear that in coordinate representation all derivatives of $\psi(x)$ participate in this relation. For the plane wave case the operator (62) is transformed simply to the factor $k/(E + m)$. It is also obvious that for a momentum small compared with the mass, equation (62) is transformed to the ordinary nonrelativistic condition of continuity of the derivatives.

3.2. Tunnelling through a constant-height barrier

The existence of the revised expressions for the current (57) and for the boundary condition (62) permits us to proceed with the description of the tunnelling phenomenon on the basis of the stationary quasi-relativistic Schrödinger-like equation (59), i.e.

$$\left(\sqrt{m^2 - \nabla^2} + V\right)\psi = E\psi. \tag{63}$$

We solve the problem of tunnelling through a constant-height barrier according to a standard scheme [13, 14], i.e. divide the space axis into three regions ($-\infty < x < 0,\ 0 < x < L,\ L < x < +\infty$, see figure 1) and find the solution to equation (63) for each of them. Then for each region we have:

$$\psi_1(x) = \exp(\mathrm{i}k_1 x) + B\exp(-\mathrm{i}k_1 x) \tag{64}$$

$$\psi_2(x) = \alpha\exp(qx) + \beta\exp(-qx) \tag{65}$$

$$\psi_3(x) = a\exp(\mathrm{i}k_1 x) \tag{66}$$

where k_1 is the initial momentum of an incident particle, and the amplitude of an incident wave equals unity. The subbarrier quasi-momentum, according to equation (63), equals

$$q = \sqrt{(2m + E^0_{\mathrm{kin}} - V_0)(V_0 - E^0_{\mathrm{kin}})}. \tag{67}$$

From the boundary condition at $x_0 = 0$ and $x_0 = L$,

$$\psi(x_0 - 0) = \psi(x_0 + 0) \tag{68}$$

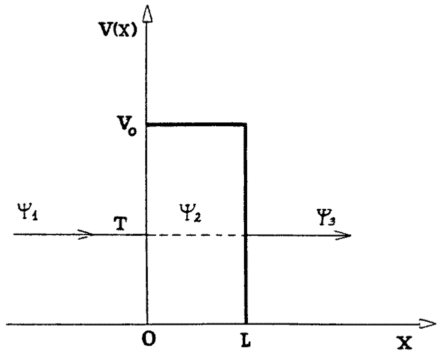

Figure 1. Potential barrier of constant height V_0; L is barrier width, $T \equiv E^0_{\rm kin}$ is the kinetic energy of an incident particle.

and its 'derivatives' (using equation (62)) we obtain four linear equations for the four unknown coefficients B, α, β, a. This set of equations is essentially the same as in the nonrelativistic case.

Our aim is to find the penetration coefficient for the barrier determined as the ratio of currents—the final (out) to the initial (incident):

$$D = \frac{j_{\rm out}}{j_{\rm in}}. \tag{69}$$

Using equation (57) we find the relevant currents

$$j_{\rm in} = \frac{k_1}{E} \qquad j_{\rm out} = a^* a \frac{k_1}{E}. \tag{70}$$

Thus, it appears that the penetration coefficient is expressed, as in the nonrelativistic case, only through the amplitude of the transmitted (out) wave

$$D = a^* a. \tag{71}$$

Then, through straightforward calculations we obtain the penetration coefficients for a barrier of constant height:

$$D_{\rm rel} = \left[1 + \left(\frac{mV_0}{k_1 q}\right)^2 \sinh^2 qL\right]^{-1} \qquad E^0_{\rm kin} < V_0 \tag{72}$$

$$D_{\rm rel} = \left[1 + \left(\frac{mV_0}{k_1}\right)^2\right]^{-1} \qquad E^0_{\rm kin} = V_0 \tag{73}$$

$$D_{\rm rel} = \left[1 + \left(\frac{mV_0}{k_1 k_2}\right)^2 \sin^2 k_2 L\right]^{-1} \qquad E^0_{\rm kin} > V_0 \tag{74}$$

where

$$k_2 = \sqrt{(E - V_0)^2 - m^2} \tag{75}$$

is the above-barrier momentum. In the nonrelativistic limit we have

$$k_1 \to k_1 = \sqrt{2mE^0_{\rm kin}} \qquad q \to q = \sqrt{2m(V - E^0_{\rm kin})} \qquad k_2 \to k_2 = \sqrt{2m(E^0_{\rm kin} - V)}$$

so that the penetration coefficients (72)–(74) reduce to the standard nonrelativistic expressions [13, 14]. The expressions (72)–(74) coincide literally with the correspondent

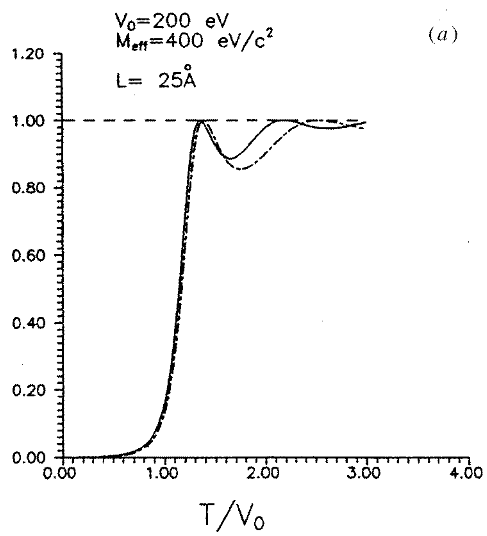

Figure 2. Dependence of the constant-height barrier penetration coefficient ($V_0 = 200$ eV, $L = 25$ Å) on the kinetic energy $T \equiv E^0_{\rm kin}$ (in units of V_0) of an incident particle of mass $m = 400$ eV c$^{-2} \simeq 0.8 \times 10^{-3}$ $m_{\rm el}$ (where $m_{\rm el}$ is the electron mass): relativistic consideration-full curve, nonrelativistic one-broken curve; (a) for the region $0 \leqslant T/V_0 \leqslant 3.0$; ($b$) for the region $0 \leqslant T/V_0 \leqslant 0.6$.

penetration coefficients from [15], where the problem has been solved by the use of the Dirac equation for a spin-up electron.

Let us give examples of calculating the penetration coefficient for different sets of parameters. To emphasize the role of relativistic effects in the tunnelling process, we take in the first example parameters which are different from the typical atomic or solid-state ones: barrier height $V_0 = 200$ eV, barrier width $L = 25$ Å and the effective mass of a tunnelling the particle $m_{\rm eff} = 400$ eV c$^{-2} \simeq 0.8 \times 10^{-3}$ $m_{\rm el}$, where $m_{\rm el}$ is the electron mass. The resulting penetration coefficients are shown in figure 2, relativistically (full curve) and nonrelativistically (broken curve), where the kinetic energy $T \equiv E^0_{\rm kin}$ of the incident particle is given on the x-axis in units of the barrier height. A more pronounced difference between the approaches to the tunnelling problem is seen in the ratio of the corresponding penetration coefficients $D_{\rm rel}/D_{\rm nonrel}$. For the same set of parameters this ratio is shown in figure 3(a) as a function of the kinetic energy of the incident particle $E^0_{\rm kin}$.

Figure 3 demonstrates that when the initial kinetic energy of the incident particle decreases, the ratio of penetration coefficients increases. This, at first sight, seems to be a paradox since it is well known that relativistic effects arise when the momentum is comparable with the particle mass. However, it becomes obvious that there is no contradiction. The point is that the difference between $D_{\rm rel}$ and $D_{\rm nonrel}$ is determined by a subbarrier quasi-momentum q which, as it follows from equation (67), increases with the decrease of the initial kinetic energy $E^0_{\rm kin}$.

The real experimental situation often satisfies the condition (quasiclassical approximation)

$$qL \gg 1 \tag{76}$$

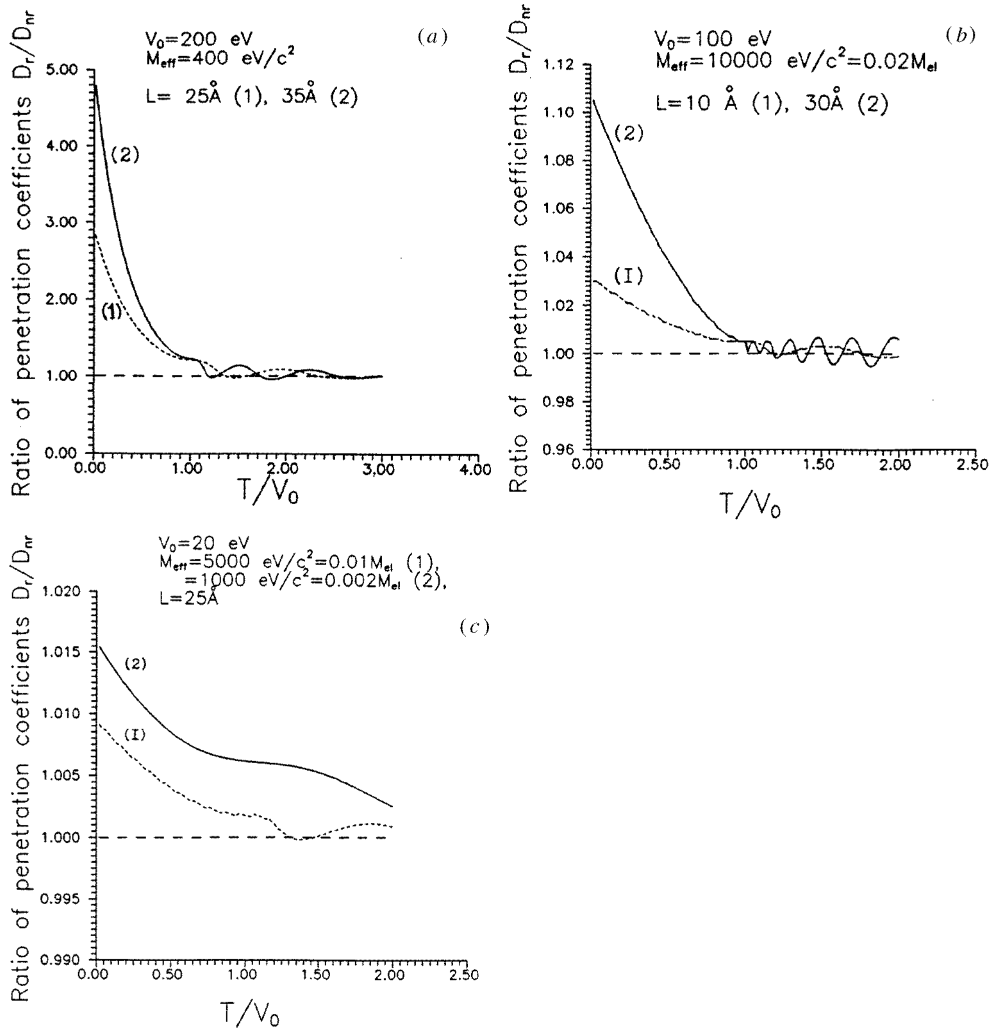

Figure 3. Penetration coefficient ratio $D_{\rm rel}/D_{\rm nonrel}$ as a function of the kinetic energy of an incident particle $T \equiv E^0_{\rm kin}$ (in units of V_0): (*a*) $V_0 = 200$ eV, $m = 400$ eV c$^{-2} \simeq 0.8\times10^{-3}\, m_{\rm el}$; $L = 25$ Å(broken curve), $L = 35$ Å(full curve). (*b*) $V_0 = 100$ eV, $m = 10^4$ eV c$^{-2} \simeq 0.02\, m_{\rm el}$; $L = 10$ Å(broken curve), $L = 30$ Å(full curve). (*c*) $V_0 = 20$ eV, $m = 5000$ eV c$^{-2} \simeq 0.01\, m_{\rm el}$ (broken curve), $m = 1000$ eV c$^{-2} \simeq 2\times10^{-3}\, m_{\rm el}$ (full curve), $L = 25$ Å.

which is realizable at $E^0_{\rm kin} << V_0$. In this case the penetration coefficient (72) is rewritten as

$$D_{\rm rel} \simeq 16\frac{E^0_{\rm kin}}{V_0}\left(1-\frac{E^0_{\rm kin}}{V_0}\right)\left(1+\frac{E^0_{\rm kin}}{2m}\right)\left(1-\frac{V_0-E^0_{\rm kin}}{2m}\right)\exp\left(-2qL\right). \quad (77)$$

In the case of an extremely small initial kinetic energy and height of the barrier in comparison with the mass of the particle, i.e. $E^0_{\rm kin} \ll m,\ V_0 \ll m$, relativistic corrections of the pre-exponential factor in equation (77) (the second and third brackets) can be neglected. Taking into account the first relativistic correction, the subbarrier quasi-momentum can be represented in the form

$$q \simeq q_{\text{nonrel}} \left(1 - \frac{V_0 - E^0_{\text{kin}}}{4m}\right) \tag{78}$$

where

$$q_{\text{nonrel}} = \sqrt{2m(V_0 - E^0_{\text{kin}})} \tag{79}$$

is the standard nonrelativistic quasi-momentum. Then, the relativistic penetration coefficient reads

$$D_{\text{rel}} \simeq D_{\text{nonrel}} \left[1 + L(V_0 - E^0_{\text{kin}})\sqrt{\frac{V_0 - E^0_{\text{kin}}}{2m}}\right]. \tag{80}$$

It follows from this expression that the relativistic corrections depend on three parameters: barrier height, V_0, barrier width, L, and particle mass, m. Figure 3 demonstrates the increase of the ratio $D_{\text{rel}}/D_{\text{nonrel}}$ with the increase of the barrier width.

It is clear that the relativistic effect results, generally, in an enhancement of the penetration ability as compared with the nonrelativistic approach. At the same time, as follows from equation (80), their ratio will be the largest when $E^0_{\text{kin}} \to 0$, i.e. when the initial kinetic energy of the incident particle decreases as compared with the barrier height V_0. This has a rather simple explanation. The relativistic phenomenon under consideration is due to relativistic values of the subbarrier quasi-momentum, q. First, q is large enough to give rise of the relativistic effects. On the other hand, it is always smaller than the nonrelativistic quasi-momentum as it is evidently seen from equation (78) and hence the relativistic penetration coefficient is always larger than the nonrelativistic one. Indeed, with making use of equation (77) we can write the ratio in the form

$$\frac{D_{\text{rel}}}{D_{\text{nonrel}}} \propto \exp\left[2L(q_{\text{nonrel}} - q)\right] = \exp\left(2Lq_{\text{nonrel}}\frac{V_0 - E^0_{\text{kin}}}{4m}\right).$$

Thus, the ratio $D_{\text{rel}}/D_{\text{nonrel}}$ goes up with decreasing initial kinetic energy of the incident particle and its maximum corresponds to zero initial kinetic energy.

Let us introduce the quantity

$$\delta_{\text{r}} = LV_0\sqrt{\frac{V_0}{2m}} \tag{81}$$

which is the maximum relative correction to nonrelativistic penetration coefficient that arises when $E^0_{\text{kin}} = 0$ (see equation (80)) and thus the maximum of $(D_{\text{rel}}/D_{\text{nonrel}})$ is $1 + \delta_{\text{r}}$. Using δ_{r}, it is possible to formulate the following critera:

- if $\delta_{\text{r}} \ll 1$, then the standard nonrelativistic approach is sufficient enough for the description of tunnelling;
- if $\delta_{\text{r}} \leqslant 1$, then the subbarrier relativistic effects should be taken into consideration in the tunnelling process.

Obviously, the nonrelativistic approximation is always applicable out of the barrier region when $E^0_{\text{kin}} \ll m$.

Examples of calculating the ratio $D_{\text{rel}}/D_{\text{nonrel}}$ for more realistic values $V_0 = 100$ eV (figure 3(*b*)) and $V_0 = 20$ eV (figure 3(*c*)) show that the subbarrier relativistic effect for atomic scales, i.e. in the standard solid state problems, leads to corrections not exceeding a few per cent.

The factor $S_b \equiv LV_0$ in equation (81) characterizes the barrier strength. We note that within the accepted system of units 1 eV $\times$ 1 Å $= \frac{1}{1973}$. But the usual atomic scales are

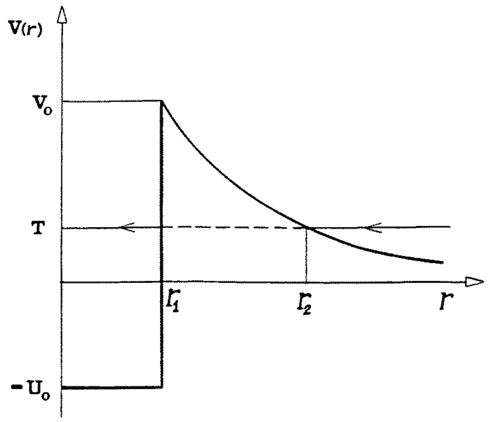

Figure 4. π^+ meson potential energy in the field of a heavy nucleus (e.g. ^{238}U): r_1 is the nuclear surface radius, r_2 is the radius at which a particle comes under the Coulomb barrier $V(r) = Ze^2/r$, i.e. $r_2 = Z\alpha/E^0_{kin}$.

$V_0 \sim 10$ eV and $L \sim 10$ Å, so that for typical solid problems $S_b \sim \frac{1}{20}$. On the other hand, it is not the case for nuclear scales where 1 MeV $\times$ 1 fm $= \frac{1}{197}$. Indeed, for typical nuclear problems $V_0 \sim 10$ MeV and $L \sim 10$ fm, so that $S_b \sim \frac{1}{2}$. Therefore, subbarrier relativistic effects are quite pronounced on the nuclear scale. In fact, it provided reason to revise the tunnelling problem in nuclear physics.

3.3. Tunnelling of positively charged particles through the Coulomb barrier of heavy nuclei

We consider the capture of a low-energy positively charged particle, for instance, a π^+ meson, by a heavy nucleus under a central collision. Three nuclei ^{207}Pb, ^{238}U and Lr^{260}Lr are taken as examples. Their nuclear plus Coulomb potential are shown schematically in figure 4. The nuclear surface radius is $r_1 = 1.4\ A^{1/3}$ fm, where A is the atomic nucleus number. Since we discuss the head-on collision of the particle with heavy nucleus, a one-dimensional approximation is applicable.

The Coulomb potential is

$$V_{\text{Coul}}(r) = \frac{Z\alpha}{r} \tag{82}$$

where Z is the number of protons in the nucleus and $\alpha = e^2 = \frac{1}{137}$. To be successful, we must take into account the relativistic corrections beyond the 'root' Hamiltonian which are due to the spatial gradients of the external field $V(r) = e\ A_0 = Z\alpha/r$. The first correction reads as (see equation (40)) $(e/8m^2)\nabla^2 A_0$ and equals zero for the Coulomb potential $A_0 = Ze/r$. We neglect corrections of higher order. Thus, for a description of the central capture of a positively charged particle by the Coulomb barrier of a heavy nucleus, we use the stationary version of equation (54) with $V = V_{\text{Coul}}(r)$.

Using the standard arguments, the penetration coefficient in quasiclassical approximation is evaluated by (the probability for the particle moving from turning point r_2 to reach the distance r_1 under the barrier)

$$D = D_0 \exp[-2\pi\eta(r_1, r_2)] \tag{83}$$

where we introduce the quantity

$$\eta(r_1, r_2) \equiv \frac{1}{\pi}\int_{r_1}^{r_2} q(r)\,\mathrm{d}r \tag{84}$$

with

$$q_{\mathrm{nonrel}}(r) = \sqrt{2m[V(r) - E^0_{\mathrm{kin}}]} \tag{85}$$

for the nonrelativistic approach and

$$q_{\mathrm{rel}}(r) = \sqrt{[2m + E^0_{\mathrm{kin}} - V(r)][V(r) - E^0_{\mathrm{kin}}]}. \tag{86}$$

for the relativistic one.

Straightforward evaluation of equation (84) results in

$$\eta(r_1, r_2) = \frac{1}{\pi}[I(r_2) - I(r_1)] \tag{87}$$

with

$$I_{\mathrm{nonrel}}(r) = r q_{\mathrm{nonrel}}(r) - \eta_0 \arcsin\left(1 - 2\frac{E^0_{\mathrm{kin}}}{V_{\mathrm{Coul}}(r)}\right) \tag{88}$$

for nonrelativistic approach and

$$\begin{aligned} I_{\mathrm{rel}}(r) = r q_{\mathrm{rel}}(r) - \gamma\eta_0 \arcsin\left(\gamma - \frac{k^2}{m V_{\mathrm{Coul}}(r)}\right) \\ - Z\alpha \arcsin\left(\gamma - \frac{V_{\mathrm{Coul}}(r)}{m}\right) \end{aligned} \tag{89}$$

for relativistic one. We have introduced above the notations

$$\eta_0 \equiv \frac{Z\alpha m}{k} = \eta(r_1 = 0, r_2) \tag{90}$$

which means the value of η when penetration through the Coulomb barrier to $r_1 = 0$ occurs; $k^2 = 2mE^0_{\mathrm{kin}}$ for the nonrelativistic approach and $k^2 = E^0_{\mathrm{kin}}(E^0_{\mathrm{kin}} + 2m)$ for the relativistic one; $\gamma = E/m$, where $E = E^0_{\mathrm{kin}} + m$ is the total energy. The radius, r_2, of a particle encountering the Coulomb barrier is determined by the kinetic energy, E^0_{kin}, of the incident particle $r_2 = Z\alpha/E^0_{\mathrm{kin}}$.

As follows from equation (77), the pre-exponential factors in both approaches at $E^0_{\mathrm{kin}} \ll m$ coincide. Therefore, the ratio $D_{\mathrm{rel}}/D_{\mathrm{nonrel}}$ will be determined by the exponential dependence only. This ratio is shown in figure 5(a) as a function of the kinetic energy of an incident π^+ meson. It is clear that at energies of the order of a few MeV, the difference can reach 20%. Thus, the capture cross section increases over that calculated by means of the nonrelativistic penetration coefficient. To estimate the effect, the same calculations are performed for the muon and the proton (the Coulomb barrier is taken in the same form as in figure 4). The results of these calculations are shown in figure 5(b) (muon) and in figure 5(c) (proton). It is seen from the graphs that for muons the effect increases, whereas for protons it is no more than 10%.

In analogy to the constant-height barrier for low-energy particles, equation (83) can be rewritten by taking into account only the first relativistic correction in the expansion of the q_{rel}, equation (86). Then the approximate penetration coefficient reads (see equation (80))

$$\tilde{D}_{\mathrm{rel}} \simeq D_{\mathrm{nonrel}}\left[1 + \int_{r_1}^{r_2}(V(r) - E^0_{\mathrm{kin}})\sqrt{\frac{V(r) - E^0_{\mathrm{kin}}}{2m}}\,\mathrm{d}r\right]. \tag{91}$$

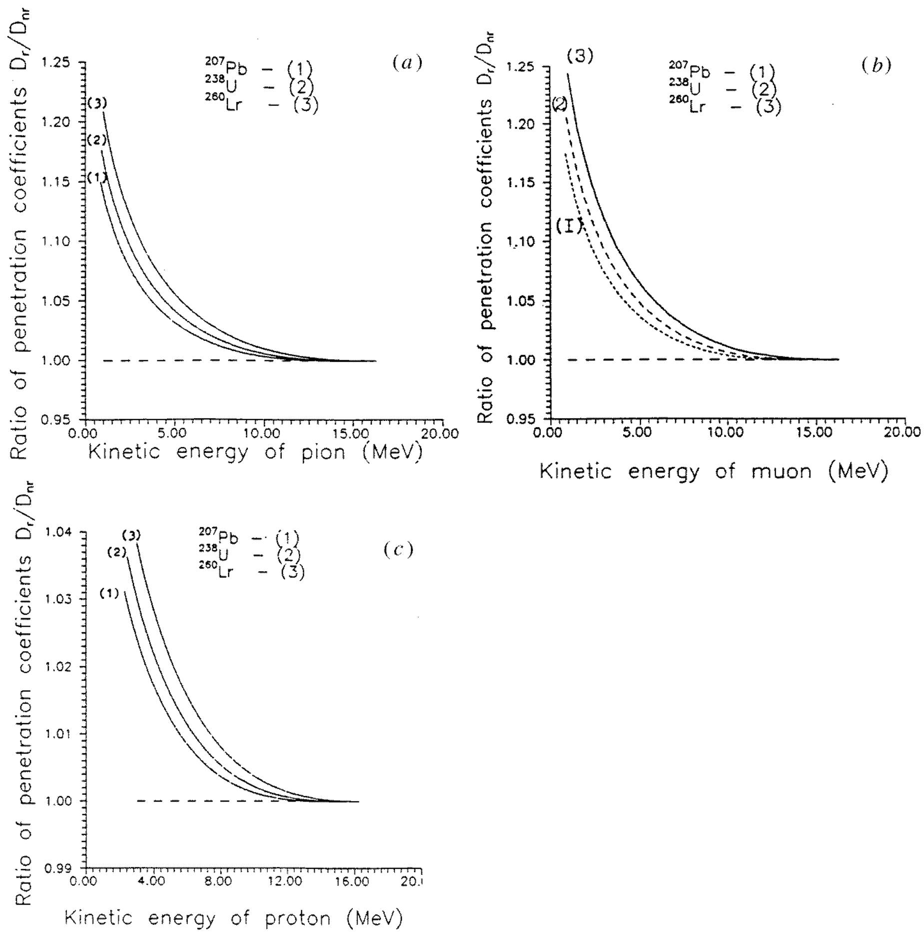

Figure 5. Penetration coefficient ratio $D_{\mathrm{rel}}/D_{\mathrm{nonrel}}$ as a function of the initial kinetic energy $T \equiv E^0_{\mathrm{kin}}$ of an incident particle. The penetration coefficient is evaluated for the Coulomb barriers of the following nuclei: ^{207}Pb-curve (1), ^{238}U-curve (2), ^{260}Lr-curve (3); (*a*) capture of π^+ meson, (*b*) capture of μ^+ meson, (*c*) capture of proton.

To verify by the pion capture example whether this approximation is good enough, we evaluated the relative error given by the approximate penetration coefficient $(D_{\mathrm{rel}} - \tilde{D}_{\mathrm{rel}})/D_{\mathrm{rel}}$, where D_{rel} is the 'exact' quantity calculated by the use of equation (89). It appears that the maximum error relative to the 'exact' relativistic penetration coefficient of the Coulomb barrier is no more than 1–3%.

Approximation (91) makes it possible as in the case of the constant height barrier, to formulate a necessary condition for taking into account the subbarrier relativistic corrections in the case of a low-energy particle tunnelling through the Coulomb barrier of a nucleus. Indeed, it is seen that a maximum relativistic effect will be observed at $E^0_{\mathrm{kin}} \to 0$, i.e. when

$$\Delta_r \equiv \int_{r_1}^{\infty} V(r)\sqrt{\frac{V(r)}{2m}}\,\mathrm{d}r = \frac{Z}{137}\sqrt{\frac{2V_0}{m}} \tag{92}$$

is comparable with unity. In equation (92), V_0 is the potential energy value on the nucleus surface $V_0 = Z\alpha/r_1$, which, for the nuclei considered, is within 14–16 MeV. Thus, if

$\Delta_r \ll 1$, the subbarrier relativistic effects can be neglected. Meanwhile, the maximum correction to the nonrelativistic penetration coefficient $\tilde{D}_{\mathrm{rel}} = D_{\mathrm{nonrel}}(1 + \Delta_r)$ in case of a central particle capture by the nucleus ^{238}U, is for π^+ mesons $\Delta_r = 0.32$, for muons $\Delta_r = 0.36$, and for protons $\Delta_r = 0.12$.

4. Summary

The Dirac and Klein–Gordon equations were examined in an external electromagnetic field. It was proved that for a special class of fields, namely $A_\nu = (A_0(t), \boldsymbol{A}(\boldsymbol{r}))$, the Dirac equation in a nonrelativistic approximation splits exactly into two Schrödinger-like equations with Hamiltonians which describe the positive and negative branches of the energy spectrum. For positive energy states the Hamiltonian has the form (36), and with a minus sign before the square root it is the Hamiltonian for negative energy states. For an arbitrary external electromagnetic field $A_\nu = (A_0(t, \boldsymbol{r}), \boldsymbol{A}(t, \boldsymbol{r}))$, the structure of the Hamiltonian is still the same except for new additional terms which are proportional to the derivatives of the electromagnetic field and represent an expansion in $1/c$. The same result was obtained for the Klein–Gordon equation, which reduces for the above special external field to the Schrödinger-like equation (51) for a wavefunction which is exactly normalized to unity. For an arbitrary external electromagnetic field additional terms appear, as in fermion case. Actually we showed that the nonrelativistic Dirac Hamiltonian

$$H_{\mathrm{D}}^{\mathrm{nonrel}} = \sqrt{m^2 + (-\mathrm{i}\boldsymbol{\nabla} - \mathrm{e}\boldsymbol{A}(t, \boldsymbol{r}))^2 - \mathrm{e}\boldsymbol{\sigma} \cdot \boldsymbol{B}(t, \boldsymbol{r})} + V(t, \boldsymbol{r}) \tag{93}$$

and the nonrelativistic Klein–Gordon one

$$H_{\mathrm{KG}}^{\mathrm{nonrel}} = \sqrt{m^2 + (-\mathrm{i}\boldsymbol{\nabla} - \mathrm{e}\boldsymbol{A}(t, \boldsymbol{r}))^2} + V(t, \boldsymbol{r}) \tag{94}$$

describe positive energy states and $V(t, \boldsymbol{r}) = \mathrm{e}A_0(t, \boldsymbol{r}) + (\mathit{truncated\ series})$ is a potential energy, where a series is an expansion in $1/c$ in combination with derivatives of the external field. On the other hand, $V(t, \boldsymbol{r})$ can be regarded as an effective or phenomenological potential energy which stands instead of the series of the relativistic corrections.

We derived the boundary conditions and expression for current for the Schrödinger equation with the Hamiltonian $H = \sqrt{m^2 - \boldsymbol{\nabla}^2} + V$. This Hamiltonian was used for a description of the tunnelling phenomenon. The particle penetration in a potential barrier of a constant height and in the Coulomb barrier were considered. It was shown that relativistic effects give an appreciable contribution to the penetration coefficient. However, for the barriers which are relevant in solid state physics the relativistic corrections are small. It is not the case on the nuclear scale. For example, the additional contribution of the relativistic corrections for penetration of the π^+ meson through the Coulomb barrier of a heavy nucleus can be around 20%. An interesting behaviour of the relativistic contribution to the penetration coefficients appears: they go up with decreasing initial kinetic energy of the incident particle. This intriguing result can be evidently understood if we consider the ratio of the penetration coefficients for the constant-height barrier in the quasiclassical approximation. In fact, with taking into account the first relativistic correction the ratio reads

$$\frac{D_{\mathrm{rel}}}{D_{\mathrm{nonrel}}} = \exp\left(2Lq_{\mathrm{nonrel}}\frac{V_0 - E_{\mathrm{kin}}^0}{4m}\right)$$

where $q_{\mathrm{nonrel}} = \sqrt{2m(V_0 - E_{\mathrm{kin}}^0)}$ and L is the barrier width (see equation (80)). Hence, the maximum of the ratio $D_{\mathrm{rel}}/D_{\mathrm{nonrel}}$ corresponds to zero initial kinetic energy.

We showed that the relativistic effects always increase the penetration coefficient which is well seen from the last equation.

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Appendix

From a combination of the Schrödinger equation (54) and its Hermitian conjugate we obtain

$$\frac{\partial \rho(t, \boldsymbol{r})}{\partial t} - \mathrm{i}\left(\psi H_0 \psi^* - \psi^* H_0 \psi\right) = 0 \tag{A1}$$

where $H_0 = \sqrt{m^2 - \nabla^2}$ and $\rho(t, \boldsymbol{r}) = \psi^*(t, \boldsymbol{r})\psi(t, \boldsymbol{r})$. Hence it follows that in the one-dimensional case the current is

$$j(t, x) = j(t, x_0) - \mathrm{i}\int_{x_0}^{x} [\psi(t, x')H_0(x')\psi^*(t, x') - \psi^*(t, x')H_0(x')\psi(t, x')]\,\mathrm{d}x'. \tag{A2}$$

If we substitute in this expression the Fourier expansion of the wavefunction into the space variable and perform explicitly the integration over x', we have

$$j(t, x) = \int\int \mathrm{d}k\,\mathrm{d}k'\,\psi(t, k)\psi^*(t, k')\frac{k + k'}{\sqrt{m^2 + k^2} + \sqrt{m^2 + k'^2}}\mathrm{e}^{\mathrm{i}(k-k')x}. \tag{A3}$$

In essence, this can be regarded as final expression for the current in momentum representation. It can be rewritten in coordinate representation in the compact form

$$j(t, x) = \left[\frac{\hat{k}(x) - \hat{k}(x')}{H_0(x) + H_0(x')}\psi(t, x)\psi^*(t, x')\right]_{x'=x}. \tag{A4}$$

The same expression can be obtained by a direct integration of equation (A2) if we represent the Hamiltonian in the form of a series.

It is obvious that in the three-dimensional case the current vector can be determined by a single given vector value—the momentum. Thus equation (A4) or (A3) will be satisfied for each component of the current vector, and equation (57) is valid. Indeed, after a Fourier expansion of the wavefunction, equation (57) transforms to

$$\begin{aligned} j_i(t, \boldsymbol{r}) &= -\frac{\mathrm{i}}{(2\pi)^6}\int\int \mathrm{d}^3k\,\mathrm{d}^3k'\,\psi(t, \boldsymbol{k})\psi^*(t, \mathbf{k}')\frac{\mathrm{i}\ (k_i + k_i')}{\sqrt{m^2 + \mathbf{k}'^2} + \sqrt{m^2 + \boldsymbol{k}'^2}}\mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot(\boldsymbol{k}-\mathbf{k}')} \\ &= -\frac{\mathrm{i}}{(2\pi)^6}\int\int \mathrm{d}^3k\,\mathrm{d}^3k'\,\psi(t, \boldsymbol{k})\psi^*(t, \boldsymbol{k}') \\ &\quad\times\frac{k_i + k_i'}{\boldsymbol{k}^2 - \boldsymbol{k}'^2}(\sqrt{m^2 + \boldsymbol{k}'^2} - \sqrt{m^2 + \boldsymbol{k}^2})\mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot(\boldsymbol{k}-\boldsymbol{k}')}. \end{aligned} \tag{A5}$$

We wish to check the expression for div $\boldsymbol{j}$. After taking derivatives of x_i and summing over i the fraction in the final integral reduces to unity, and we finally obtain

$$\begin{aligned}\operatorname{div} \boldsymbol{j}(t, \boldsymbol{r}) &= -\mathrm{i} \int\int \mathrm{d}^3 k \, \mathrm{d}^3 k' \, \psi(t, \boldsymbol{k}) \psi^*(t, \boldsymbol{k}') (\sqrt{m^2 + \boldsymbol{k}'^2} - \sqrt{m^2 + \boldsymbol{k}^2}) \mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot(\boldsymbol{k}-\boldsymbol{k}')} \\ &= -\mathrm{i}(\psi H_0 \psi^* - \psi^* H_0 \psi) \end{aligned} \tag{A6}$$

as has to be obtained by equation (A1).

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