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RELATIVISTIC VERSION OF THE TRANSFER MATRIX METHOD

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Abstract
One derives the relativistic version of the transfer matrix method for an electron moving through a piecewise constant potential.
Keywords: Dirac equation, Transfer matrix method

1. Introduction

The simplest non-relativistic quantum modeling of nanoscale semiconductor devices is based on the Schrödinger equation written in solid state domains where the potential is constant and the influence of the lattice is encapsulated in the value of effective electron mass. When the devices are made from semiconductor heterostructures, there are many such domains separated among themselves by interfaces where besides the step in potential we also have to consider the discontinuity in effective electron mass [1]. The problem has been solved by applying appropriate boundary conditions [2],

$$\psi_L = \psi_R, \quad \frac{1}{m_L}\frac{\partial \psi_L}{\partial x} = \frac{1}{m_R}\frac{\partial \psi_R}{\partial x}, \tag{1}$$

where ψ_L, m_L and ψ_R, m_R are the electron wave function and effective mass of the electron to the left (L) and right (R) side of a given interface. The results obtained with the above-described procedure are in agreement with experimental data [3] and are widely used since the transmission coefficient can be calculated via the simple method of the transfer matrix [4,5]. However, the assumed boundary conditions (1) are imposed somewhat artificially in order to conserve the particle current.

Another attitude is to start with the Dirac equation even though it is clear that the relativistic effects have to be very small. Nevertheless, the relativistic linear dependence between

energy and mass could offer some technical advantages for finding appropriate connection conditions at interfaces where the potential and the effective mass present discontinuities [6].

Our purpose is to derive the relativistic version of the transfer matrix method for the motion in a fixed direction of a Dirac electron with point-dependent effective mass, passing through rectangular barriers of arbitrary profile. We show that the use of the Dirac equation allows one to impose simple connection prescriptions at interfaces. However, the price to pay for working with variable mass is that there are many energy scales corresponding to different mass values. For this reason we need to rescale the experimental potential if we want to measure the energies with respect to a unique energy scale. The rescaled potential will be considered the appropriate relativistic potential of our problems. We show that only in this way the non-relativistic limit of our approach recovers the results derived from Schrödinger equation with the conditions (1).

2. Plane waves. One dimensional motion

Let us consider the Minkowski space-time in a frame of coordinates x^μ ($\mu,\nu,... = 0,1,2,3$) and the metric $\eta = \mathrm{diag}(1,-1,-1,-1)$. In natural units (with $\hbar = c = 1$) the time is $x^0 = t$ while the space coordinates, $x^1 = x$, $x^2 = y$ and $x^3 = z$, are the components of the vector $\vec{x}$. In this frame, the relativistic quantum motion of an electron of mass m and charge $-e$, in an arbitrary external electromagnetic field A_μ, is governed by the Dirac equation [7],

$$\gamma^\mu(i\partial_\mu - eA_\mu)\psi - m\psi = 0, \tag{2}$$

that produces the conserved current (in units of $-e$): $j^\mu = \overline{\psi}\gamma^\mu\psi$, where $\overline{\psi} = \psi^+\gamma^0$ is the Dirac adjoint of the spinor ψ. In what follows, we take the γ-matrices in the standard representation (with diagonal γ^0) [7]. Here we are interested to study the quantum modes in the particular case of a space domain D where $\vec{A}(x) = 0$ and $eA_0(x) = V = \text{const.}$ for any $\vec{x} \in D$. In this domain the Dirac equation can be analytically solved and different quantum modes can be well-defined using complete sets of commuting operators. Thus the plane wave solutions are eigenspinors of the complete set of commuting operators $\{E_D, \vec{P}, W\}$ constituted by the Dirac operator, $E_D = i\gamma^\mu\partial_\mu - \gamma^0 V$, momentum $\vec{P} = i\nabla$, and the Pauli-Lubanski operator $W = 2\vec{P}\cdot\vec{S}$. The

corresponding eigenvalues, m, $\vec{k}$ and λ, define the plane wave spinor of positive frequency, momentum $\vec{k}$, energy $E(\vec{k}) = \sqrt{m^2 + \vec{k}^2} + V$ and helicity λ that reads [7,8]

$$\psi_{\vec{k},\lambda}(x) = \frac{1}{\sqrt{2m}} \begin{pmatrix} \sqrt{E(\vec{k}) - V + m}\ \xi_\lambda(\vec{k})(4) \\ \lambda\sqrt{E(\vec{k}) - V - m}\ \xi_\lambda(\vec{k}) \end{pmatrix} e^{-iE(\vec{k})t + i\vec{k}\cdot\vec{x}} \tag{3}$$

We denoted by $\xi_\lambda(\vec{k})$ the normalized Pauli spinors of the helicity basis that satisfy $\vec{k}\cdot\vec{\sigma}\xi_\lambda(\vec{k}) = \lambda|\vec{k}|\xi_\lambda(\vec{k})$ and $[\xi_\lambda(\vec{k})]^+\xi_{\lambda'}(\vec{k}) = \delta_{\lambda,\lambda'}$ (where σ_i are the Pauli matrices and $\lambda = \pm 1$). One can verify that each solution (3) is normalized as $\overline{\psi}_{\vec{k},\lambda}\psi_{\vec{k},\lambda'} = \delta_{\lambda,\lambda'}$ and, along the direction $\vec{k}$ produces the current $j = \frac{1}{|\vec{k}|}\overline{\psi}_{\vec{k},\lambda}(\vec{k}\cdot\vec{\gamma})\psi_{\vec{k},\lambda} = \frac{|\vec{k}|}{m}$, (4)

The general results presented above help us to write down the solutions of simpler one-dimensional problems along the third axis. Of a special interest is the problem of the electron moving through a system of N rectangular barriers of arbitrary shape (Fig. 1). These domains are limited by plane interfaces at fixed points, $z_1, z_2, ..., z_{N+1}$, among them those from z_1 and z_{N+1} represent the interfaces between the system of barriers and the domains outside, denoted by $D_{in} \equiv D_0 = (-\infty, z_1]$ and, respectively, $D_{out} \equiv D_{N+1} = [z_{N+1}, \infty)$. It is natural to consider that in these latter domains the potential vanishes, $V_{in} = V_{out} = 0$. In addition, we assume that in each domain D_i the electron has the *effective* mass m_i while in the domains D_{in} and D_{out} its mass is just the *bare* mass m.

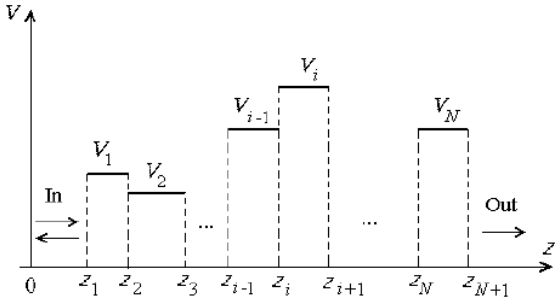

Figure 1 A sequence of potential steps

In special relativity the energy scale depends on the value of the rest mass while the electromagnetic potential is defined up to a gauge. Therefore, in problems where this mass is

replaced by a point-dependent effective mass, we could introduce a *unique* energy scale only by choosing suitable gauge fixings, dealing with the different values of the effective mass. In these conditions we are encouraged to consider in each domain D_i the *relativistic* potential $\hat{V}_i$ instead of the experimental one V_i. The relation among these potentials has to be derived from a natural supplemental condition which will fix up the gauge in the domains D_i.

In any domain D_i there exists a plane wave solution of energy E and helicity λ propagating in the sense of the positive semiaxis z,

$$\phi^i_{E,\lambda}(t,z) = \frac{1}{\sqrt{2m_i}} \begin{pmatrix} k_i^{(+)} \xi_\lambda \\ \lambda k_i^{(-)} \xi_\lambda \end{pmatrix} e^{-iEt+ik_i z}, \tag{5}$$

which depends on the constants $k_i^{(\pm)} = \sqrt{E - \hat{V}_i \pm m_i}$ and scalar momentum

$$k_i = k_i^{(+)} k_i^{(-)} = \sqrt{(E-\hat{V}_i)^2 - m_i^2}. \tag{6}$$

We note that in this case the helicity spinors coincide to those of the spin basis since the spin is projected on the third axis. Consequently, the two-component spinors ξ_λ take the usual form $\xi_1 = (1,0)^T$ and $\xi_{-1} = (0,1)^T$. The plane wave solution with the same E and λ but propagating in the opposite sense reads

$$\chi^i_{E,\lambda}(t,z) = \frac{1}{\sqrt{2m_i}} \begin{pmatrix} k_i^{(+)} \xi_\lambda \\ -\lambda k_i^{(-)} \xi_\lambda \end{pmatrix} e^{-iEt-ik_i z}. \tag{7}$$

The conclusion is that, in a domain D_i, the most general plane wave solutions of energy E and helicity λ are given by the linear combinations

$$\Psi^i_{E,\lambda}(t,z) = A_i \phi^i_{E,\lambda}(t,z) + B_i \chi^i_{E,\lambda}(t,z), \tag{8}$$

where A_i and B_i are arbitrary complex numbers. Each solution (8) gives the total current which does not depend on helicity:

$$j_i = \frac{k_i}{m_i}\left(|A_i|^2 - |B_i|^2 \right), \tag{9}$$

Finally we can establish the relation among the relativistic and experimental potentials assuming that in a domain D_i the momentum k_i vanishes only when the total non-relativistic energy $E_{nr} = E - m$, calculated with respect to the bare mass m, equals the experimental potential V_i. Therefore, according to Eq. (6) we obtain the form of our relativistic potentials

$$\hat{V}_i = V_i + \delta m_i , \tag{10}$$

where $\delta m_i = m - m_i$.

3. The transfer matrix

In what follows we shall derive the transfer matrix in the pure scattering case. This means that the energy satisfies the condition $E \geq E_0 = \sup\{V_i + m | i = 0,1,...,N+1\}$ and k_i take only real values. In addition, we specify that the global solutions we consider here have the same fixed energy E and helicity λ in all the domains D_i. In problems involving many domains D_i it is difficult to manipulate solutions of the form (8). For this reason we replace these solutions by *associated* two-dimensional vectors [4, 6],

$$v_i(z) = \begin{pmatrix} A_i e^{ik_i z} \\ B_i e^{-ik_i z} \end{pmatrix}, \tag{11}$$

which carry all the information we need for calculating the currents (10):

$$j_i = \frac{k_i}{m_i}[v_i(z)]^+ \sigma_3 v_i(z), \quad \forall z \in D_i . \tag{12}$$

Thus the vectors (11) become the basic elements of the relativistic formalism of the transfer matrix for rectangular barriers [5]. In the domains D_0 and D_{N+1}, where the potential vanishes and the mass is m, the spinors $\Psi^0_{E,\lambda}$ and $\Psi^{N+1}_{E,\lambda}$ are associated to the vectors:

$$v_{in}(z) \equiv v_0(z) = \begin{pmatrix} A_{in} e^{ikz} \\ B_{in} e^{-ikz} \end{pmatrix}, \qquad v_{out}(z) \equiv v_{N+1}(z) = \begin{pmatrix} A_{out} e^{ikz} \\ B_{out} e^{-ikz} \end{pmatrix}. \tag{13}$$

Now, the problem is to find the transfer matrix, M, which transforms the *out* vector into the *in* one as

$$v_0(z_1) = M\, v_{N+1}(z_{N+1}), \tag{14}$$

allowing one to calculate the transmission coefficient. The global solution of energy E and helicity λ is continuous in each point z_i which means that:

$$\Psi^{i-1}_{E,\lambda}(t, z_i) = \Psi^{i}_{E,\lambda}(t, z_i) \tag{15}$$

for $i = 1,2,...,N+1$. After a few manipulations we find that these conditions lead to simple relations among the associated vectors,

$$v_{i-1}(z_i) = M_i v_i(z_i), \quad i = 1,2,...,N+1, \tag{16}$$

where the matrices

$$M_i = \frac{1}{2}\begin{pmatrix} r_i^{(+)} + r_i^{(-)} & r_i^{(+)} - r_i^{(-)} \\ r_i^{(+)} - r_i^{(-)} & r_i^{(+)} + r_i^{(-)} \end{pmatrix}, \quad r_i^{(+)} = \sqrt{\frac{m_{i-1}}{m_i}}\frac{k_i^{(+)}}{k_{i-1}^{(+)}}, \quad r_i^{(-)} = \sqrt{\frac{m_{i-1}}{m_i}}\frac{k_i^{(-)}}{k_{i-1}^{(-)}}. \tag{17}$$

The last step is to introduce the translation matrices

$$T_i = \begin{pmatrix} e^{ik_i(z_{i+1}-z_i)} & 0 \\ 0 & e^{-ik_i(z_{i+1}-z_i)} \end{pmatrix} \tag{18}$$

which transform $v_i(z_i)$ into $v_i(z_{i+1}) = T_i v_i(z_i)$. With these elements we can write down the final expression of the *relativistic* transition matrix

$$M = \left[\prod_{i=1}^{N} M_i T_i\right] M_{N+1}. \tag{19}$$

For $E \geq E_0$, when k_i are real numbers, the matrices $M_i = M_i^+$ and have the property

$$M_i \sigma_3 M_i = r_i^{(+)} r_i^{(-)} \sigma_3 = \frac{m_{i-1}}{k_{i-1}}\frac{k_i}{m_i}\sigma_3 \tag{20}$$

which guarantees the conservation of the total current (12), $j_{in} = j_1 = ... = j_i = ... = j_{out}$. In these circumstances, taking $B_{out} = 0$ we have $|A_{in}|^2 - |B_{in}|^2 = |A_{out}|^2$ which allows us to define the transmission coefficient

$$T = \frac{|A_{out}|^2}{|A_{in}|^2} = |M_{11}|^{-2}. \tag{21}$$

We note that T results to be a function only of energy, being independent on the helicity of the electron passing through the rectangular barriers. The function $T(E)$ calculated here is defined only on the domain $E \geq E_0$. However, starting with the present theory, the extension to energies smaller than E_0 can be done but this is no trivial because of the wells producing discrete energy levels or tunnelling effects which need to be treated with specific methods.

Conclusions

Here we constructed the relativistic version of the transfer matrix for the Dirac electron moving through rectangular barriers, in a similar manner as in the non-relativistic theory based on the Schrödinger equation. Our approach allows one to calculate the transfer matrices using the same rules but with matrices M_i of different forms.

In the non-relativistic limit the quantities $k_i^{(-)} = \sqrt{E_{nr} - V_i}$ remain unchanged but we have $k_i^{(+)} \to \sqrt{2m_i}$. Consequently, we find that $r_i^{(+)} \to 1$ remaining with the terms

$$r_i^{(-)} = r_i = \sqrt{\frac{m_{i-1}}{m_i} \frac{E_{nr} - V_i}{E_{nr} - V_{i-1}}}, \tag{22}$$

which *coincide* to those of Refs. [5] at least in the domain $E \geq E_0$ considered here. Thus, the general conclusion is that the non-relativistic limit of our approach based on the three-dimensional Dirac equation with the relativistic potentials (10) reproduces identically the results of the traditional method based on the Schrödinger equation and conditions (1).

In other respects, the results obtained here indicate that the use of the Dirac equation could be helpful in other problems concerning the motion of electrons in semiconductor heterostructures as suggested in Ref. [6].

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