Applying the Dirac equation to derive the transfer matrix for piecewise constant potentials

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One propose a relativistic version of the transfer matrix method for an electron moving through a given number of rectangular barriers of arbitrary shape. It is shown that starting with the Dirac equation depending on the effective mass and a suitably chosen relativistic potential, one obtains a relativistic transfer matrix which takes the correct traditional form in the non-relativistic limit.

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I. INTRODUCTION

The recent advances in nanostructure technology allow the fabrication of electronic devices which inherently experience quantum effects in their operation. There is a need for theoretical tools, not only to understand the behavior of actual nanoscale devices, but also to initiate future research and developments.

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]. In the ’60 the problem has been solved by applying appropriate boundary conditions [2].

Let us consider the Minkowski space-time in a frame

\[ (\mu, \nu, \ldots) = (0, 1, 2, 3) \]

and charge

\[ e \]

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 \( A_\mu \), is governed by the Dirac equation [7],

\[ \gamma^\mu(i\partial_\mu - eA_\mu)\psi - m\psi = 0 \],

II. PLANE WAVES

Let us consider the Minkowski space-time in a frame of coordinates \( x^\mu (\mu, \nu, \ldots = 0, 1, 2, 3) \) and the metric \( \eta = \text{diag}(1, -1, -1, -1) \). 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 \( A_\mu \), is governed by the Dirac equation [7],

\[ \gamma^\mu(i\partial_\mu - eA_\mu)\psi - m\psi = 0 \],

where \( \psi_L, m_L \) and \( \psi_R, m_R \) 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 and the method is widely used in electron transport computations through semiconductor heterostructures [4]. The advantage of this model is that the transmission coefficient can be calculated using the simple and elegant method of the transfer matrix [4, 5]. However, the assumed boundary conditions [1] are imposed somewhat artificially in order to conserve the particle current without to have a deeper physical motivation.

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. Few years ago, the one-dimensional Dirac equation was successfully used for treating problems with variable mass avoiding several difficulties of the non-relativistic theory [6].

In this paper we would like to continue this study using the normalized plane wave solutions of the three-dimensional Dirac equation in helicity basis. 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 an 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].

The paper is organized as follows. In the second section we present the well-known plane wave solutions of the Dirac equation in the helicity basis. The next section is devoted to the problem of one-dimensional rectangular barriers of any shape allowing us to find the relativistic transfer matrix in section four. Finally, it is shown that in the non-relativistic limit this matrix becomes just the desired traditional one [3].
that produces the conserved current (in units of $-e$)

$$j^\mu = \bar{\psi} \gamma^\mu \psi,$$  

(3)

where $\bar{\psi} = \psi^\dagger \gamma^0$ is the Dirac adjoint of the spinor $\psi$. In what follows, we take the $\gamma$-matrices in the standard representation (with diagonal $\gamma^0$).

Here we are interested to study the quantum modes in the particular case of a space domain $D$ where $\hat{A}(x) = 0$ and $eA_0(x) = V = \text{const.}$ for any $x \in D$. 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 $\lambda$, define the plane wave spinor of positive frequency, momentum $\vec{k}$, energy $E(\vec{k}) = \sqrt{m^2 + \vec{k}^2 + V}$ and helicity $\lambda$ that reads

$$\psi_{\vec{k},\lambda}(x) = \frac{1}{\sqrt{2m}} \left( \frac{\sqrt{E(\vec{k}) - V + m} \xi_\lambda(\vec{k})}{\lambda \sqrt{E(\vec{k}) - V - m} \xi_\lambda(\vec{k})} \right) \times e^{-iE(\vec{k})t + ik \cdot \vec{x}}.$$  

(4)

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

$$j = \frac{1}{|\vec{k}|} \bar{\psi}_{\vec{k},\lambda} (\vec{k} \cdot \vec{\gamma}) \psi_{\vec{k},\lambda} = \frac{|\vec{k}|}{m},$$  

(5)

along the direction $\vec{k}$.

III. ONE-DIMENSIONAL MOTION

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. In general, the system of barriers is constituted by $N$ domains $D_i = [z_i, z_{i+1}]$ where the potential $V(z)$ takes constant values $V_i$ (Fig.1). These domains are limited by plane interfaces at fixed points, $z_1, z_2, \ldots, z_N, z_{N+1}$, 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 $m$.

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 an 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 $V_i$ 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 $\lambda$ propagating in the sense of the positive semiaxis $z$,

$$\phi^i_E,\lambda(t, z) = \frac{1}{\sqrt{2m_i}} \left( \frac{k^{(+)\dagger}_i \xi_\lambda}{\lambda k^{(-)\dagger}_i \xi_\lambda} \right) e^{-iEt + ik_i z},$$  

(6)

which depends on the constants $k^{(+)\dagger}_i = \sqrt{E - V_i \pm m_i}$ and scalar momentum

$$k_i = k^{(+)\dagger}_i k^{(-)\dagger}_i = \sqrt{(E - V_i)^2 - m_i^2}.$$  

(7)

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 $\xi_\lambda$ take the usual form $\xi_1 = (1, 0)^T$ and $\xi_{-1} = (0, 1)^T$. The plane wave solution with the same $E$ and $\lambda$ but propagating in the opposite sense reads

$$\chi^i_E,\lambda(t, z) = \frac{1}{\sqrt{2m_i}} \left( \frac{k^{(+)\dagger}_i \xi_\lambda}{\lambda k^{(-)\dagger}_i \xi_\lambda} \right) e^{-iEt - ik_i z}.$$  

(8)

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

$$\Psi^i_E,\lambda(t, z) = A_i \phi^i_E,\lambda(t, z) + B_i \chi^i_E,\lambda(t, z),$$  

(9)

where $A_i$ and $B_i$ are arbitrary complex numbers. Each solution $\psi$ gives the total current

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

(10)
which does not depend on helicity.

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. (12) we obtain the form of our relativistic potentials

\[ \hat{V}_i = V_i + \delta m_i, \]

where \( \delta m_i = m - m_i \).

IV. THE TRANSFER MATRIX

In what follows we shall derive the transfer matrix in the pure scattering case without wells or tunneling effects. 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 potential vanishes and the mass is \( m \) respect to the bare mass \( m \).

The last step is to introduce the translation matrices

\[ T_i = \begin{pmatrix} e^{-ik_i(z_{i+1} - z_i)} & 0 \\ 0 & e^{ik_i(z_{i+1} - z_i)} \end{pmatrix}, \]

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

\[ M = \prod_{i=1}^{N} M_i T_i M_{N+1}. \]

The global solution of energy \( E \) and helicity \( \lambda \) is continuous in each point \( z_i \) which means that we must impose the conditions

\[ \Psi_{E,\lambda}^{-1}(t, z_i) = \Psi_{E,\lambda}(t, z_i) \]

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

\[ v_{i-1}(z_i) = M_i v_i(z_i), \quad i = 1, 2, ..., N + 1, \]

where the matrices

\[ M_i = \frac{1}{2} \begin{pmatrix} r_i^{(+)} + r_i^{(-)} & r_i^{(+)} - r_i^{(-)} \\ r_i^{(+)} - r_i^{(-)} & r_i^{(+)} + r_i^{(-)} \end{pmatrix} \]

depend on the constants

\[ r_i^{(+)} = \sqrt{\frac{m_{i-1}}{m_i}} k_i^{(+)} \quad r_i^{(-)} = \sqrt{\frac{m_{i+1}}{m_i}} k_i^{(-)}. \]

We note that \( \delta m_i = m_i - m \), calculated according to Eq. (18) have the property

\[ M_i \sigma_3 M_i^* = r_i^{(+)} r_i^{(-)} \sigma_3 = \frac{m_{i-1}}{m_i} \]

which guarantees the conservation of the total current, \( j_{in} = j_1 = ... = j_i = ... = j_{out} \), calculated according to Eq. (13). 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

\[ T = \frac{|A_{out}|^2}{|A_{in}|^2} = |M_{11}|^{-2}. \]

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.

Of course, 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 requires specific treatment because of the wells producing discrete energy levels or tunneling effects which need to be treated with specific methods.
V. 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.

Let us see what happens with our theory in the non-relativistic limit, for small values $E_{nr} - V_i \ll m_i$. In this limit the quantities $k_i^(-) = \sqrt{E_{nr} - V_i}$ remain unchanged but we have $k_i^(+)$ tend to $\sqrt{2m_i}$. Consequently, we find that $r_i^(-) = r_i = \sqrt{\frac{m_{i-1}}{m_i} \frac{E_{nr} - V_i}{E_{nr} - V_{i-1}}}$, (25)

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 [11] reproduces identically the results of the traditional method based on the Schrödinger equation and conditions [1]. Moreover, relativistic corrections can be also calculated but so far these seem to be small in the usual regime the electronic devices work.

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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