THE TRANSPORT OF THE DIRAC FERMIONS THROUGH CERTAIN ONE-DIMENSIONAL QUANTUM WIRE STRUCTURES

D.M. BALTAȚEANU
West University of Timisoara, Faculty of Physics, Bd. V. Pârvan, No. 4, RO-300223, Timisoara, Romania, e-mail: doru.baltateanu@e-uvt.ro

Received September 2, 2015

The relativistic transport through semiconductor-based quantum wires in electric field is investigated, using a relativistic extension of the transfer matrix. The effects of the position-dependent effective mass and the electric field on transmission are analyzed and some comments on oscillatory behavior of the relative difference between the relativistic and the non-relativistic coefficients are made.

Key words: Dirac equation, quantum wire, relativistic transfer matrix.

1. INTRODUCTION

In the last years, the low-dimensional systems have become a very interesting place of research in which new theories and models for studying the optoelectronic properties are proposed, many of them being verified by modern experiments [1]. Due to the recent advances of technologies, now it becomes possible to create even single channels for propagation that can be considered as one-dimensional quantum wires, in which the electrons are confined to move along one direction [2, 3].

The electronic transport through low-dimensional semiconductors systems has been intensively studied using the non-relativistic quantum mechanics, which is a powerful tool for understanding the behavior and the properties of such structures [4]. However, in some instances one can use the relativistic formalism, especially for spin-dependent transport in which the spin effects must be highlighted, even the relativistic corrections are small.

There are fewer suggestive examples when the relativistic theory is successfully used in condensed matter, avoiding some difficulties that could appear in the non-relativistic one [5–7]. In Ref. [8], starting from the complete (1+3) Dirac equation, a relativistic version of the transfer matrix for piecewise constant potentials has been proposed. Also, using the Dirac equation, the persistent current in an isolated Aharonov-Bohm ring has been calculated and some type of anomaly has been revealed, due to the electron spin [9].
The transport of Dirac fermions through certain one-dimensional quantum wire-structures

Therefore, under certain circumstances, even at low energies the use of the relativistic theory is justified because could lead to new effects that does not exist or remain hidden in the non-relativistic theory.

Being motivated of the above mentioned studies, we propose a computational model in which the relativistic transmission through two quantum-wire structures in uniform electric field is investigated. The paper is structured as follows. In Section 2 the relativistic transmission coefficient and the relative difference between this coefficient and the non-relativistic one are numerically computed, using the transfer matrix method for piecewise potentials. The obtained results are presented in Section 3 and the concluding remarks are given in Section 4.

2. THEORETICAL MODEL

Consider an one-dimensional (1D) and ideal quantum wire composed by three alternating semiconductor layers, in which the Dirac electron is restricted to move only along the z-axis, with the spin projected to this direction. The Dirac equation (in a frame $x^\nu$, $\nu = 0, 1, 2, 3$) is:

$$\gamma^\nu \left[ i\hbar \partial_{\nu} - (e/c) A_{\nu} \right] \psi - m_0 \psi = 0$$

In Eq. (1) $\Psi$ represents the Dirac spinor, $\gamma^\nu$ are the Dirac matrices and $(\hbar, e, m_0, c)$ are the Planck constant, the electron charge, the bare electron mass and the light velocity, respectively. $A^\nu$ is the electromagnetic potential that incorporates the effects of the electric and magnetic fields.

In our case the ideal wire is exposed to an external and uniform electric field so that the vector potential $A = 0$ and the scalar potential is constant. Since the electric field is constant the spin flips does not exist. We shall assume that the transport is ballistic (without scattering) and there are no electron-electron interactions. The reason of these simplifications is to highlight the combined effects of the position-dependent effective mass and of the electric field, respectively.

The quantum point contacts (junctions) between the quantum wire layers are simulated by three barriers with a certain potential profile. We select two potential profiles corresponding to the quantum-wire structures denoted by QWR$_1$ (Fig. 1a) and QWR$_2$ (Fig. 1b). These will be used to make comparisons regarding the effect of the position-dependent effective mass on the relativistic transmission coefficient in the absence/presence of the external field.

In Fig. 1 the IN/OUT domains represent the entrance/exit from structures. In the absence of the bias voltage, the potential is $V(z) = 0$ for $z \in (-\infty, 0) \cup [z_3, +\infty)$ and $V_i$ for $z \in [z_{i-1}, z_i)$, ($i = 1, 2, 3$). Note that for QWR$_1$, $V_1 < V_2 < V_3$ and for QWR$_2$, $V_2 = V_3$.
For the biased structures, the potential is \( V(z) = 0 \) for \( z \in (-\infty, 0] \), \( V_i - (V_i/L)z \) for \( z \in [z_{i-1}, z_i) \) and \( V(z) = -V_a \) for \( z \in [z_i, +\infty) \). \( L = z_3 \) is the total length of the structures and \( V_a = e \cdot U_a \) is the potential introduced by the voltage \( U_a \). In the IN/OUT domains the effective masses are \( m_i = m_{out} = m_0 \) and in the barriers the effective masses are \( m_i^* \), that changes at the passing from one barrier to another.

Regarding the QWR\(_2\) structure, for \( z \in [z_1, z_3] \) and for energies in the domain \([V_2, V_1]\) (Fig. 1b) the relativistic electron can be reflected back and forth from barriers 1 and 3, like in a quantum well. If its energy matches the values of the resonant levels in the well, a perfect transmission occurs and the quantum system becomes totally transparent.

These model choices allow us to analyzing different behaviors of the relativistic transmission coefficient. Simultaneously, we expect that in certain energy range, a switch of the transmission could be performed (one of the structures to be in the ON state \( (T_r = 1) \) and the other in the OFF state \( (T_r = 0) \)).

In order to use the relativistic extension of the transfer matrix for piecewise potentials, the whole domain for \( z \in (z_0, z_3) \) is divided into a number of smaller sub-domains \( p \in \mathbb{N}^* \) with the length \( L/p \), in which the potential can be regarded as a constant. In any sub-domain \( j (j = 1 \ldots p) \) the plane wave solutions are vectors of the form [9]:

\[
\xi_j(z) = \begin{pmatrix} A_j e^{ik_j z} \\ B_j e^{-ik_j z} \end{pmatrix},
\]

where \( A_j \) and \( B_j \) are complex amplitudes and \( k_j \) are wave vectors given by:

\[
k_j = \left( \left(E_{rel} - V_{rel,j} \right)^2 - m_{j*}^2 \cdot c^4 \right)^{1/2} / hc
\]

Fig. 1 – Two different profiles of potential in the quantum wire: (a) QWR\(_1\), with \( V_1 < V_2 < V_3 \); (b) QWR\(_2\), with \( V_1 = V_3 > V_2 \); the bold lines represent the potential for a bias voltage \( U_a \).
In Eq. (3) $E_{\text{rel}} = E + m_0c^2$ is the relativistic energy (E represents the non-relativistic energy) and $V_{\text{rel},j} = V_j + (m_0-m_0^*)c^2$ is the relativistic potential, introduced to preserve the zero-level of the non-relativistic energy to the same value [9]. We stress that one needs to introduce this potential due to the position-dependent effective mass.

In the presence of the bias voltage, the potentials for IN/OUT domains are $V_{\text{in}} = 0$, $V_{\text{out}} = -V_a$ and the relativistic potential reads:

$$V_{\text{rel},\text{in}} = (m_0-m_0^*)c^2; \quad V_{\text{rel},\text{out}} = -V_a + (m_0-m_0^*)c^2.$$  (4)

The corresponding wave vectors are as follows:

$$k_{\text{in}} = \left[ E_{\text{rel}}^2 - m_0^2c^4 \right]^{1/2}/hc; \quad k_{\text{out}} = \left[ (E_{\text{rel}} + V_a)^2 - m_0^2c^4 \right]^{1/2}/hc.$$  (5)

Additionally, the plane wave solutions are identified by the vectors:

$$\xi_{\text{in}}(z) = \left( A_{\text{in}}e^{ik_{\text{in}}z} \quad B_{\text{in}}e^{-ik_{\text{in}}z} \right)^T; \quad \xi_{\text{out}}(z) = \left( A_{\text{out}}e^{ik_{\text{out}}z} \quad B_{\text{out}}e^{-ik_{\text{out}}z} \right)^T,$$  (6)

with $A_{\text{in}} = 1$, $B_{\text{in}} = r$, $A_{\text{out}} = t$ and $B_{\text{out}} = 0$, $r$ and $t$ being the reflection and the transmission amplitudes, respectively (superscript $T$ stands for matrix transpose).

The vectors $\xi_{\text{in}}$ and $\xi_{\text{out}}$ are connected through a total relativistic transfer matrix:

$$M = \left( \prod_{j=1}^{p} M_j N_j \right) M_{\text{out}}.$$  (7)

In Eq. (7) $M_j$ are transfer matrices that connect the vectors $\xi_{j+1}(z_{j-1})$ and $\xi(z_{j-1})$, $N_j$ are transporting matrices that connect the vectors $\xi(z_{j+1})$ and $\xi(z_j)$, and $M_{\text{out}}$ is a transfer matrix that connects the vectors $\xi_{p}(z_{p})$ and $\xi_{\text{out}}(z_{p})$.

The matrices $M_j$ are given by:

$$M_j = \frac{1}{2} \begin{pmatrix} r_j^+ + r_j^- & r_j^+ - r_j^- \\ r_j^+ - r_j^- & r_j^+ + r_j^- \end{pmatrix},$$  (8)

with

$$r_j^= \sqrt{\left(m_j^+ / m_j^- \right) \cdot \left(k_j^2 / k_{j+1}^2 \right)}; \quad k_j^= \sqrt{\left(E_{\text{rel},j} \pm m_j^+c^2 \right)/hc}.$$  (9)
The transporting matrices $N_j$ are given by:

$$N_j = \begin{pmatrix} e^{-ik_j L_j} & 0 \\ 0 & e^{ik_j L_j} \end{pmatrix}, \quad \text{with } L_j = z_j - z_{j-1}. \quad (10)$$

The relativistic transmission coefficient $T_r$ is calculated using the expression:

$$T_r = \frac{k_{out}}{k_{in}} \cdot \frac{1}{|M_{11}|^2}, \quad (11)$$

where $M_{11}$ is the element (1,1) of the total transfer matrix $M$.

Finally, numerical calculations of the non-relativistic transmission coefficient $T_{nr}$ are carried out by means of the well-known non-relativistic transfer matrix for piecewise potentials [4] and a comparison between both transmission coefficients is performed, using the relative difference $D = (T_r - T_{nr})/T_{nr}$.

### 3. NUMERICAL RESULTS AND DISCUSSIONS

Here we study the behavior of the relativistic coefficient $T_r$ and of the relative difference $D$, focusing on the effect of the position-dependent effective mass on the transmission in unbiased/biased structures.

For both quantum-wire structures, the barriers are alternating Al$_x$Ga$_{1-x}$As layers with different Al molar concentrations and the IN/OUT domains are GaAs layers. The effective mass in barriers is position-dependent and in the IN/OUT domains $m_{in} = m_{out} = m_0 = 0.067m_e$. The conduction-band discontinuity between GaAs and Al$_x$Ga$_{1-x}$As is sensitive to the Al percentage and in our model is $\Delta E_c = 1.1x$ for $0 \leq x \leq 0.45$ [10].

For QWR$_1$ we select three different values for the $x$ fraction, $x_1 = 0.2$, $x_2 = 0.3$ and $x_3 = 0.4$, corresponding to the potentials $V_1 = 0.22eV$, $V_2 = 0.33eV$ and $V_3 = 0.44eV$. In this case the effective masses in Al$_x$Ga$_{1-x}$As layers are $m_1^{*} = 0.0836m_e$, $m_2^{*} = 0.0919m_e$ and $m_3^{*} = 0.1002m_e$. For QWR$_2$ the selected values of the $x$ fraction are $x_1 = x_3 = 0.35$, $x_2 = 0.2$, obtaining the potentials $V_1 = V_3 = 0.385eV$ and $V_2 = 0.22eV$. The corresponding effective masses are $m_1 = m_3 = 0.09605m_e$ and $m_2 = 0.0836m_e$.

#### 3.1. THE RELATIVISTIC TRANSMISSION THROUGH THE UNBIASED QUANTUM STRUCTURES

We start by studying the dependence of the transmission coefficients and of the relative difference, respectively, on the electron energy in the absence of the bias voltage. The corresponding graphs are illustrated in Fig. 2, in which both regimes, $E < \min (V_i)$ (tunneling) and $E > \max (V_i)$ (scattering) are considered.
First, it can be observed that the plots for the transmission coefficients \( T \) and \( T_{nr} \) (Fig. 2a and 2c) coincide. In this energy range the relativistic corrections are small and, consequently, the values of the transmission coefficients are superposed. Anyway, this confirms the accuracy of our computational method, for unbiased structures.

In the scattering domain the transmission shows an oscillatory behavior for both structures. When the reflected wave is completely eliminated (due to the interference effects), a perfect transmission occurs and transmission peaks appear, as we can see in Fig. 2a and 2c. These peaks are slowly broadened as the energy increases, being affected by the position-dependent effective mass, which induces an asymmetry in the potential profile. Our results agree with those obtained in the non-relativistic approach (using models with transfer matrix or Airy functions) for different multi-barrier systems [11–13].

In the tunneling domain, between 0.22 eV and 0.385 eV one can observe that the QWR\(_1\) structure is totally opaque (Fig. 2a) but in the QWR\(_2\) structure resonance states occur (Fig. 2c). There are four line-type transmission peaks (very sharp, with a very small width) for which the QWR\(_2\) structure is totally transparent.

For obtaining these resonance peaks a searching algorithm has been used, with an energy step \( \Delta E = 10^{-16} \) eV. The numerical values of the resonance energies are \( E_{r1} = 0.22809 \) eV, \( E_{r2} = 0.25219 \) eV, \( E_{r3} = 0.29153 \) eV and \( E_{r4} = 0.34372 \) eV. We specify that for a potential quantum device designed with these structures, in the above energy range, if \( E = E_{ri} (i = 1...4) \) a switch from the QWR\(_2\) state with \( T_r = 1 \) (ON state) to a state with \( T_r = 0 \) (OFF state-in QWR\(_1\)) could be done.

The relative difference \( D \) has an interesting behavior, being very sensitive at the potential profile in the barriers (Figs. 2b and 2d). For both structures, at small tunneling energies (\( E < 0.22 \) eV) \( D \) vanish when the energy increases. For \( E > 0.22 \) eV, in the QWR\(_1\) structure an oscillations regime appears and \( D \) reaches the zero value at certain energies. This type of behavior has been also revealed in our previous paper [14] for a single biased barrier, but in this case the shape of oscillations is quite different, due to the effect of asymmetry introduced by the values of the barriers heights.

We note that for the QWR\(_2\) configuration, from 0.22 eV to 0.385 eV, the relative difference \( D \) is not plotted due to the discrete values \( E_{ri} (i = 1...4) \) which are isolated points. \( D \) is in fact proportional with the derivative of the transmission and does not make sense in these points. Theoretically, when the electron energy matches the exact values of the resonance energies, the resonant tunneling occurs (\( T_r = T_{nr} = 1 \)) and the relative difference \( D = 0 \). Because the peaks have a very small width, around the resonance energies, for \( E = E_{ri} \pm \Delta E \) (\( \Delta E \to 0 \)) both transmission coefficients vanish rapidly.
However, in our calculations there is a small difference between $T_r$ and $T_{nr}$ coefficients. If we employ the search algorithm with a high resolution to obtain energies that almost match with the resonance values $E_{ri}$, one of the coefficients jumps to a value very close to unity. Because the resonant peaks are very sharp, the other coefficient jumps to a very small value. For example, if $\Delta E = 10^{-16}$ eV, for $E = 0.2915352034176$ eV $\sim E_{ri}$, $T_r \sim 0.9997$ and $T_{nr} \sim 5.72 \times 10^{-6}$. For another value $E' = 0.2915352390651$ eV, with $E'-E = 3.56 \times 10^{-8}$ eV, $T_{nr}$ jumps to a value of 0.9999 and $T_r$ vanishes ($T_r \sim 5.73 \times 10^{-6}$). This happens for all resonance energies $E_{ri}$ in the specified energy spectrum.

3.2. THE RELATIVISTIC TRANSMISSION IN THE BIASED QUANTUM STRUCTURES

In Fig. 3 the relativistic transmission coefficient function on the electron energy is illustrated for both structures, at two different bias voltages and for a
number of sub-domains \( p = 2400 \). We can see that in the presence of the electric field the line-type resonance peaks for the QWR\(_2\) structure are suppressed (Fig. 3b).

![Graph showing relativistic transmission versus electron energy for biased QWR\(_1\) and QWR\(_2\) structures](image)

Using the searching algorithm for \( U_a = 100 \text{ mV} \), the energies associated to these peaks have been obtained, with the values 0.176 eV, 0.203 eV, 0.242 eV and 0.293 eV. The associated values for the relativistic coefficient are 1.13 \( \times 10^{-6} \), 5.17 \( \times 10^{-3} \), 5.15 \( \times 10^{-3} \) and 2.5 \( \times 10^{-4} \), respectively. Comparing these values with those for unbiased structure, it is clear that the four line-type peaks are much diminished and shifted towards lower energies, this being a signature of the electric field. Obviously, this shifting towards lower energy takes place for all the transmission peaks, for both quantum structures.

If the voltage increases at \( U_a = 250 \text{ mV} \), the positions of the peaks are again shifted but this shifting is more substantially for QWR\(_1\) (solid line in Fig. 3a). It can be observed that from 0.2 eV to 0.35 eV the transmission peaks are maintained at high values in QWR\(_1\), being suppressed in QWR\(_2\). For certain voltages, adjusting the energy values in the above domain, QWR\(_1\) can be in ON state and QWR\(_2\) in OFF state. For example, at \( U_a = 250 \text{ mV} \), for \( E \approx 0.23 \text{ eV} \), QWR\(_1\) is totally transparent and QWR\(_2\) is totally opaque (see solid lines in Fig. 3a and 3b).

The different shapes of the transmission curves for both configurations are due to the interplay between the position-dependent effective mass and the applied field. Our results are in agreements with those presented in other papers, in which a numerical method based on the transfer matrix in the non-relativistic formalism is used [11, 15].
Next, the dependences of the relativistic transmission coefficient and the relative difference on the bias voltage are presented in Fig. 4, for two fixed values of the incident energy.

![Graph](image)

**Fig. 4** – The relativistic transmission and the relative difference *versus* the voltage for QWR$_1$ (a, b) and QWR$_2$ (c, d); the dashed and solid lines correspond to $E = 0.36$ eV and $E = 0.37$ eV; $p = 2400$.

We see again that the shape of the transmission curves for QWR$_1$ is totally different compared to those for QWR$_2$. For the first structure, the increasing of the voltage after a critical value leads to a significant increasing of the transmission and to apparition of transmission peaks (Fig. 4a). For $E = 0.36$ eV (dashed line in Fig. 4a) the first transmission peak appears close to 110 mV and for $E = 0.37$ eV this peak is shifted towards a lower voltage ($\approx 95$ mV) and is diminished (solid line in Fig. 4a).

This shifting towards lower voltages appears also in the QWR$_2$ configuration (Fig. 4c). For $E = 0.36$ eV the peaks are much suppressed and are not clearly visible on the graph; only one peak that appears at 179 mV can be observed (the dashed line in Fig. 4c). Increasing energy at the value 0.37 eV, the transmission
The transport of Dirac fermions through certain one-dimensional quantum wire-structures

peaks are shifted to lower voltages and tend to increase, being visible on the graph (solid line in Fig. 4c).

Based on these results, we can observe that using adequate values for the energy, one can adjust the voltage in a range for which one structure can be totally (or partially) transparent and the other totally (or partially) opaque (or vice versa).

Concerning the relative difference, for both configurations this exhibits the same features like the derivative of the transmission. For voltages lower than the critical value, $D$ is very small (between $10^{-12}$ and $10^{-9}$) and above the critical value has an oscillatory behavior, with a maximum amplitude of the order $10^{-4}$ (Figs. 4b and 4d). At the increasing of the electron energy (from 0.36 eV to 0.37 eV) these oscillations are also shifted towards lower voltages and have different amplitudes, depending on the field intensity.

4. CONCLUSIONS

Our model represents an application of the formal theory presented in Ref. [8], being an alternative for computing the transmission through quantum wires with position-dependent effective mass. The relativistic transmission coefficient is numerically computed over the whole energy spectrum (tunneling and scattering), with a good numerical accuracy and compared with the non-relativistic coefficient. For energy values in the scattering range, the relative difference between the coefficients exhibits an oscillatory behavior, with oscillations that are very sensitive at the variation of the electric field.

The selected quantum wires configurations represents a clear example in which the position-dependent effective masses in combination with the external field have a strong effect on the relativistic transmission. The behavior of our selected structures suggests that one could construct special quantum devices with semiconductor wires, in which the transmission can be controlled in various ways. However, this is not an easy task but could be possible due to the advances of the modern technologies [3].

The model is simplified in order to reveal the effects of the asymmetry on the transmission but it can be easy generalized for more barriers with different potential profiles. Also it can be considered as a starting point for other models with more realistic configurations of quantum wires exposed to electric and magnetic fields, in which the spin polarization effects could be considered.

Acknowledgements. D.M. Baltateanu is supported by the strategic grant POSDRU/159/1.5/ S/137750, Project Doctoral and Postdoctoral programs support for increased competitiveness in Exact Sciences research, cofinanced by the European Social Fund within the Sectoral Operational Programme Human Resources Development 2007–2013.
REFERENCES