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Electronic transmission through p–n and n–p–n junctions of graphene

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Abstract
In this paper, we first evaluate the electronic transmission of Dirac fermions into a p–n junction of gapped graphene and show that the final result depends on the sign of the refractive index, n. We also, by considering the appropriate wavefunctions in the region of the electrostatic potential, show that both transmission and the reflection probability turn out to be positive and less than unity instead of the negative transmission and higher than unity reflection coefficient commonly referred to as the Klein paradox. We then obtain the transmission probability corresponding to a special p–n junction for which there exists a region in which the low energy excitations of graphene acquire a finite mass and, interestingly, find that in this case the transmission is independent of the index of refraction, in contrast with the corresponding result for gapped graphene. We then discuss the validity of the solutions reported in some of the papers cited in this work which, considering the Büttiker formula, turn out to lead to the wrong results for conductivity.

1. Introduction

Graphene, i.e. carbon atoms one atom thick arranged into a honeycomb structure, has attracted much attention since it was isolated for the first time in 2004 [1]. The main reasons for this attention are graphene's intriguing physics for fundamental research and its potential applications for future nano-electronics devices such as graphene nano-transistors. Here, it should be noted that the energy dispersion relation of graphene was first studied by Wallace [2]. In fact the energy spectrum of graphene is linear in momentum (just like the energy spectrum of photons) so that the conduction and valence bands of the graphene spectrum touch in two inequivalent points, referred to as *Dirac points* in the first Brillouin zone, resulting in four degenerate modes. This close resemblance of low energy excitations of graphene to ultra-relativistic particles, requires a relativistic dynamic equation to describe their electronic transport in this material. One can, therefore, obtain such an equation from the tight binding model, which turns out to be the following massless Dirac-like equation:

$$v_F \boldsymbol{\sigma} \cdot \mathbf{p}\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{1}$$

where $v_F \approx 10^6$ m s^{-1} is the Fermi velocity of massless Dirac fermions of graphene and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y)$, with σ^i, $i = x, y, z$, the i Pauli matrix. Note that the existence of massless Dirac fermions in graphene [3–5] has been demonstrated experimentally [6, 7], and therefore the above equation really describes the behavior of its charge carriers. Thus, some quantum-field theoretical problems, such as the so-called Klein paradox [8], can be put to the test in this one atom thick carbon material.

In this paper, in the next section, we study the scattering of Dirac fermions from a p–n junction of gapped graphene and show that the transmission probability depends on the sign of the refractive index (or equivalently on the band index in the region of the electrostatic potential). We then calculate the transmission for a special potential step of height V_0 under which electrons acquire a finite mass, due to the presence of a gap of 2Δ in the graphene spectrum [9] which results in changing of its energy spectrum from the usual linear dispersion to a hyperbolic energy dispersion relation, and find that the probability is independent of the band index. We then show that, using the appropriate wavefunctions for an electron with energy $E < V_0$ incident perpendicularly on a potential step of height V_0, one can arrive at positive and smaller than one values for transmission and reflection probabilities,

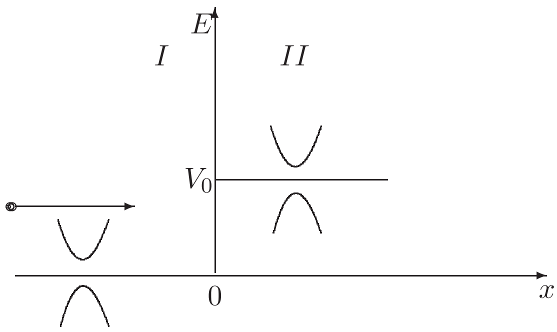

Figure 1. An electron of energy E incident upon a p–n junction of gapped graphene.

respectively, and therefore the pair creation phenomenon commonly associated with this effect is disregarded.

Here, we note that one of the methods for inducing finite gaps in energy spectra of graphene is to grow it on top of a hexagonal boron nitride with the B–N distance very close to the C–C distance of graphene [10]. In this way, it is possible to build up some regions in graphene where its energy spectrum reveals a finite gap, meaning that charge carriers there behave as massive Dirac fermions while there can be still regions where massless Dirac fermions are also present. In this work, by considering this possibility we also investigate the tunneling of electrons with energy E into an electrostatic barrier of height V_0 which allows quasi-particles to acquire a finite mass in a region where the dispersion relation of graphene exhibits a parabolic spectrum and find that it is not completely transparent even when the resonance condition is satisfied, in contrast with the usual n–p–n junctions that, in this case, exhibit total transparency. However, this is not the end of the story. In section 4.1, we also discuss some incorrect results found in the expression for the reflection coefficient and transmission probability, T, obtained in [11] and [12] and then show that considering the appropriate wavefunction in the region of the electrostatic potential gives us a more reasonable expression for transmission probability. We also briefly discuss some other models and obtain transmission at the normal incidence and in the limit of no electrostatic potential [13]; however, in this case graphene does not meet negative refraction [14], such as tunneling of the electrons into a p–n junction under a perpendicular magnetic field [15], or an electrostatic potential. However, in [16] the carrier density in the p–n junction is locally controlled by electrostatic gating and therefore graphene can meet the negative refraction. At the end of this section we note that in graphene n–p–n and p–n junctions could correspond to a potential barrier and a potential step, respectively, if they are sharp enough [17].

2. Tunneling in gapped graphene through a p–n junction

In this section we study the massive electrons tunneling into a two-dimensional (2D) potential step (n–p junction) of a gapped graphene which shows a hyperbolic energy spectrum unlike the linear dispersion relation of a pure graphene (see figure 1). Here, the low energy excitations, therefore, are governed by the 2D massive Dirac equation. Thus, in order to calculate the transmission probability, we first need to obtain the eigenfunctions of the following Dirac equation which describes the Dirac fermions in gapped graphene:

$$H = v_F \boldsymbol{\sigma} \cdot \mathbf{p} + \Delta\sigma^z, \tag{2}$$

where 2Δ is the induced gap in the graphene spectrum and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y)$ with

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3}$$

are the Pauli vector matrices. Now for obtaining the corresponding eigenfunctions of Hamiltonian (2) one may rewrite it as

$$H = \begin{pmatrix} \Delta & v_F|\mathbf{p}|e^{-i\varphi_\mathbf{p}} \\ v_F|\mathbf{p}|e^{i\varphi_\mathbf{p}} & -\Delta \end{pmatrix}, \tag{4}$$

where

$$\varphi_\mathbf{p} = \arctan(p_y/p_x). \tag{5}$$

As one can readily see, the corresponding eigenvalues are given by:

$$E = \lambda\sqrt{\Delta^2 + v_F^2 p^2}, \tag{6}$$

where $\lambda = \pm 1$ corresponds to the positive and negative energy states, respectively. Now in order to obtain the eigenfunctions, one can make the following ansatz:

$$\psi_{\lambda,\mathbf{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} u_\lambda \\ v_\lambda \end{pmatrix} e^{i(k_x x + k_y y)}, \tag{7}$$

where we have used units such that $\hbar = 1$. Plugging the above spinors into the corresponding eigenvalue equation then gives u_λ and u_λ as

$$u_\lambda = \sqrt{1 + \frac{\lambda\Delta}{\sqrt{\Delta^2 + v_F^2 k^2}}}, \qquad v_\lambda = \lambda\sqrt{1 - \frac{\lambda\Delta}{\sqrt{\Delta^2 + v_F^2 k^2}}}\, e^{i\varphi_k}. \tag{8}$$

Now that the corresponding eigenfunctions of Hamiltonian (2) have been found, assuming an electron incident upon a step of height V_0, we can write the single valley Hamiltonian as follows[3]:

$$H = v_F \boldsymbol{\sigma} \cdot \mathbf{p} + \Delta\sigma^z + V(\mathbf{r}), \tag{9}$$

where $V(\mathbf{r}) = 0$ for region I ($x < 0$) and for region II ($x > 0$), massive Dirac fermions feel an electrostatic potential of height

[3] The Hamiltonian corresponding to the other Dirac point is obtained by replacing Δ by $-\Delta$.

V_0 with kinetic energy $E - V_0$. The wavefunctions in the two regions then are given by:

$$\psi_{\rm I} = \frac{1}{\sqrt{2}}\begin{pmatrix}\alpha\\ \gamma\lambda e^{i\phi}\end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}}\begin{pmatrix}\alpha\\ \gamma\lambda e^{i(\pi-\phi)}\end{pmatrix} e^{i(-k_x x + k_y y)} \tag{10}$$

and

$$\psi_{\rm II} = \frac{t}{\sqrt{2}}\begin{pmatrix}\beta\\ \lambda'\eta e^{i\theta_t}\end{pmatrix} e^{i(q_x x + k_y y)}, \tag{11}$$

where r and t are reflected and transmitted amplitudes, respectively, $\lambda' = \pm 1$ is the band index and $\phi = \arctan(\frac{\mathbf{k}_y}{\mathbf{k}_x})$ is the angle of propagation of the incident electron wave[4] and $\theta = \arctan(\frac{\mathbf{k}_y}{\mathbf{q}_x})$ with

$$\mathbf{q}_x = \pm q_x = \pm\sqrt{\left[\frac{(V_0 - E)^2 - \Delta^2}{v_F^2}\right] - k_y^2} \tag{12}$$

the propagation angle of the transmitted electron wave[5]. Here we emphasize that $\mathbf{q}_x$ takes its positive (negative) value when $E > V_0$ ($E < V_0$), since the group velocity has a relation with the momentum vector

$$v_{\rm group} = \frac{dE}{d\mathbf{q}}, \tag{13}$$

that must be positive (negative) for the former (latter) case. Keeping this in mind, however, in what follows, for convenience we no longer use our unconventional notations $\mathbf{a}_i$ (where $a = k, q$ and $i = x, y$). From the above discussion, we find that θ_t, which is the angle of the momentum vector relative to the x-axis, in the case of $E > V_0$ is the same as the propagation angle of the wavefunction, i.e. $\theta_t = \theta$, while in the case of $E < V_0$, we have $\theta_t = \theta + \pi$. Note that in order to make things as simple as possible, we have introduced the following abbreviations:

$$\alpha = \sqrt{1 + \frac{\lambda\Delta}{\sqrt{\Delta^2 + v_F^2(k_x^2 + k_y^2)}}}, \qquad \gamma = \sqrt{1 - \frac{\lambda\Delta}{\sqrt{\Delta^2 + v_F^2(k_x^2 + k_y^2)}}}, \tag{14}$$

$$\beta = \sqrt{1 + \frac{\lambda'\Delta}{\sqrt{\Delta^2 + v_F^2(q_x^2 + k_y^2)}}}, \qquad \eta = \sqrt{1 - \frac{\lambda'\Delta}{\sqrt{\Delta^2 + v_F^2(q_x^2 + k_y^2)}}}. \tag{15}$$

[4] So, one considers ϕ to be restricted to the interval $[-\pi/2, \pi/2]$. Note that $\mathbf{k}_x = +k_x$, since the electron is assumed to be incident upon the step from the left.

[5] With this definition, θ, the refraction angle (or equivalently the angle of the group velocity vector measured from the normal incidence) falls in the interval $[-\pi/2, \pi/2]$. For example, for a material with a negative index of refraction [14], in the case of $\mathbf{k} = (k_x, -k_y)$ ($\mathbf{k} = (k_x, -k_y)$), we get $\theta > 0$ ($\theta < 0$).

Now, imposing the continuity conditions of $\psi_{\rm I}$ and $\psi_{\rm II}$ at the interface $x = 0$, leads to the following system of equations:

$$\alpha + \alpha r = \beta t, \tag{16}$$

$$\lambda\gamma e^{i\phi} - \lambda\gamma r e^{-i\phi} = \lambda'\eta t e^{i\theta_t}, \tag{17}$$

and solving them with respect to the reflection probability, R, gives

$$R = \frac{N_r - 2\lambda\lambda' S_r \cos(\phi - \theta_t)}{N_r + 2\lambda\lambda' S_r \cos(\phi + \theta_t)}, \tag{18}$$

where N_r and S_r are

$$N_r = \frac{\beta^2\gamma^2 + \alpha^2\eta^2}{\beta^2\gamma^2} = 2\frac{E|V_0 - E| - \lambda\lambda'\Delta^2}{(|V_0 - E| + \lambda'\Delta)(E - \lambda\Delta)} \tag{19}$$

and

$$S_r = \frac{\alpha\eta}{\beta\gamma} = \frac{(|V_0 - E| + \lambda'\Delta)(E - \lambda\Delta)}{(|V_0 - E| - \lambda'\Delta)(E + \lambda\Delta)}. \tag{20}$$

Now it is obvious that in the limit $\Delta \to 0$ we get the same reflection as that of the massless case and in the limit of no electrostatic potential we arrive at the logical result $R = 0$. This is important because, as we will see later, for a special potential step in this limit, R is not zero. Also note that for normal incidence we get

$$R(0) = \frac{N_r - 2S_r}{N_r + 2S_r}. \tag{21}$$

Now one remaining problem is to calculate the transmission probability. Considering the equations (16) and (17) and the fact that the x-component of the probability current j_x is constant in the two regions I and II, so that

$$j_x^{in} = \lambda\alpha\gamma\cos\phi, \qquad j_x^r = -\lambda\alpha\gamma|r|^2\cos\phi, \qquad j_x^t = \lambda'\eta\beta|t|^2\cos\theta_t, \tag{22}$$

T is found to be

$$T = |t|^2\frac{\lambda\lambda'\eta\beta\cos\theta_t}{\alpha\gamma\cos\phi} \tag{23}$$

or equivalently can be written as

$$T(\phi) = \frac{4\lambda\lambda' S_t\cos\phi\cos\theta_t}{N_t + 2S_t\lambda\lambda'\cos(\phi + \theta_t)}, \tag{24}$$

where

$$S_t = \frac{\eta\beta}{\alpha\gamma} = \frac{q}{k}\frac{E}{|V_0 - E|}, \tag{25}$$

and

$$N_t = \frac{\eta^2\alpha^2 + \beta^2\gamma^2}{\alpha^2\gamma^2} = 2\frac{E(E|V_0 - E| - \lambda\lambda'\Delta^2)}{v_F^2 k^2|V_0 - E|}. \tag{26}$$

As is clear, the probability T is not simply given by $|t|^2$. Physically the fact that T is not given by $|t|^2$ is because in the conservation law:

$$\nabla\cdot\mathbf{j} + \frac{\partial}{\partial t}|\psi|^2 = 0, \tag{27}$$

which gives the following relation for the probability current:

$$\mathbf{j} = v_F \psi^\dagger \boldsymbol{\sigma} \psi, \tag{28}$$

it is the probability current that matters, which is not simply given by the probability density $|\psi|^2$. It also contains the velocity which means that if the velocity changes between the incoming wave and the transmitted wave, T is not, therefore, given by $|t|^2$, although the ratio of the two velocities enters the calculations. At this point an interesting result is revealed. Considering an electron approaching perpendicularly to the step, one can obtain $T(0)$ as follows:

$$T(0) = 2\frac{v_F^2|k_x||q_x|}{E|V_0 - E| - \lambda\lambda'\Delta^2 + v_F^2|k_x||q_x|}. \tag{29}$$

which shows that transmission because of the appearance of $\lambda\lambda'\Delta^2$ depends on the sign of the refractive index n, whereas the transmission, in the limit $\Delta \to 0$, which corresponds to the expression for the tunneling of massless electrons in pure graphene, is independent of whether the refractive index is positive or negative. In other words, the probability in gapped graphene contrary to pure graphene depends on the band indexes, λ and λ'. Therefore it is revealed that the conductivity of the gapped graphene, considering expression (24) and the Büttiker formula [18] (see equation (81)), depends on the band index as well.

We also see that in the case of $V_0 \to 0$ and $V_0 \to \infty$, one arrives at $T = 1$. Also note that in the limit of $\Delta \to 0$, as

$$E|V_0 - E| = v_F^2|k_x||q_x|, \tag{30}$$

we see that probability reaches unity in agreement with the result obtained for pure graphene.

3. Tunneling through a p–n junction of graphene

In this section we consider the scattering of an electron of energy E from a potential step of height V_0 which allows massless electrons to acquire a finite mass in the region of the electrostatic potential (see figure 2). The p–n junction considered here is such that there exists a finite gap for $x > 0$ with an electrostatic potential of height V_0. Thus, in order to calculate the transmission probability of the charge carriers for which the electrostatic potential is given by

$$V(\mathbf{r}) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0, \end{cases} \tag{31}$$

we have to consider two different wavefunctions, one corresponding to the region $x < 0$ and another to a region of finite gap. Therefore, assuming an electron of energy E, propagating from the left, the wavefunctions then in the first and second domains are

$$\psi_I = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \lambda e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}}\begin{pmatrix} 1 \\ \lambda e^{i(\pi-\phi)} \end{pmatrix} e^{i(-k_x x + k_y y)}, \tag{32}$$

and

$$\psi_{II} = \frac{t}{\sqrt{2}}\begin{pmatrix} \beta \\ \lambda'\eta e^{i\theta} \end{pmatrix} e^{i(q_x x + k_y y)}, \tag{33}$$

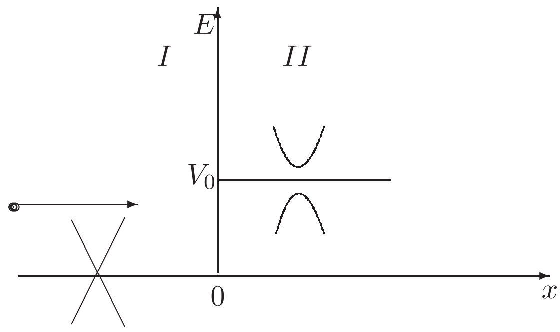

Figure 2. A massless electron of energy E incident on a p–n junction of height V_0.

where for some reasons that we will explain later, in ψ_{II}, θ is the propagation angle and not, as it should be, the angle that the momentum vector makes relative to the x-axis, i.e. θ_t. So, applying the continuity condition of the wavefunctions at $x = 0$ yields

$$1 + r = \beta t, \tag{34}$$

$$\lambda e^{i\phi} - r\lambda e^{-i\phi} = \lambda'\eta t e^{i\theta}. \tag{35}$$

Now, by solving the above equations we arrive at the following expressions for tt^* and R

$$tt^* = \frac{2\cos^2\phi}{1 + \lambda\lambda'\eta\beta\cos(\phi+\theta)} \tag{36}$$

$$R = rr^* = \frac{1 - \lambda\lambda'\eta\beta\cos(\phi-\theta)}{1 + \lambda\lambda'\eta\beta\cos(\phi+\theta)} \tag{37}$$

where

$$\eta\beta = \left[\frac{v_F^2(q_x^2 + k_y^2)}{v_F^2(q_x^2 + k_y^2) + \Delta^2}\right]^{\frac{1}{2}} < 1. \tag{38}$$

As θ is the propagation angle, equation (37) implies that the reflection coefficient exceeds unity for an electron of energy $E < V_0$, since in this case $\lambda\lambda' = -1$. Therefore, θ must be replaced by $\theta_t = \theta + \pi$. Before we discuss this result, note that using the probability conservation law, one can show that the probability T is given by $T = \frac{\lambda\lambda'\eta\beta\cos\theta}{\cos\phi}|t|^2$ and therefore it can be expressed as

$$T = \frac{2\lambda\lambda'\eta\beta\cos\theta\cos\phi}{1 + \lambda\lambda'\eta\beta\cos(\phi+\theta)}. \tag{39}$$

We see that in the limit $\Delta \to 0$ one arrives at the following solution for T:

$$T = \frac{2\lambda\lambda'\cos\theta\cos\phi}{1 + \lambda\lambda'\cos(\phi+\theta)} \tag{40}$$

which seems to be the transmission of massless Dirac fermions through a p–n junction in gapless graphene. Equation (40) shows that in the case of $E > V_0$, T is positive and also less than unity, whereas in the case of $E < V_0$, we find that the probability is negative and for normal incidence tends to infinity.

This negative T and higher than one reflection probability that equations (40) and (37) imply, arise from this fact that we did not consider the appropriate direction of the momentum vector in $\psi_{\rm II}$. As we discussed earlier, the direction of the group velocity and momentum, in this case, are opposite and therefore θ in (33) must be replaced by θ_t. In other words in the case of $E < V_0$, the phase of the wavefunction in momentum space undergoes a π change in transmitting from region I to region II or equivalently the direction of $\mathbf{q}$ rotates by 180°, so that the directions of the group velocity and $\mathbf{q}$ become opposite under the potential step. Hence instead of equations (40) and (37) we can write

$$T(\phi) = \frac{2\eta\beta\lambda\lambda' \cos\theta_t \cos\phi}{1 + \eta\beta\lambda\lambda' \cos(\phi + \theta_t)},$$
$$R(\phi) = \frac{1 - \eta\beta\lambda\lambda' \cos(\phi - \theta_t)}{1 + \eta\beta\lambda\lambda' \cos(\phi + \theta_t)}. \tag{41}$$

These expressions now reveal that both transmission and reflection probability are positive and less than unity. Therefore the pair creation that commonly is regarded as an explanation for the appearance of the negative values for T is completely disregarded (see [22]). Note that, one arrives at negative values for transmission probability merely because of confusing the direction of the group velocity, $\mathbf{v}_q$, with the direction of $\mathbf{q}$ or equivalently—from a 2D point of view—the propagation angle with the angle that the momentum vector under the electrostatic potential makes with the normal incidence. So the π phase change of the transmitted wavefunction in momentum space under the electrostatic potential (in the case of $E < 0$) must be considered.

Also note that for normal incidence we have

$$T(0) = \frac{2\eta\beta}{1+\eta\beta} = \frac{v_{\rm F} q_x}{|V_0 - E| + v_{\rm F} q_x},$$
$$R(0) = \frac{1-\eta\beta}{1+\eta\beta} = \frac{|V_0 - E| - v_{\rm F} q_x}{|V_0 - E| + v_{\rm F} q_x} \tag{42}$$

which shows that the transmission, contrary to the result obtained in the previous section for gapped graphene, is independent of the sign of the refractive index. The reader may have noticed that this independence is not limited to the normal incidence, since for $\lambda' = -1$ we have $\theta_t = \theta + \pi$ while for $\lambda' = 1$ the propagation angle and the transmission angle are the same, i.e. $\theta_t = \theta$. So, for equal values of $|V_0 - E|$ regardless of band index, equation (41) gives the same values for probability. In the limit $V_0 \gg E \approx \Delta$ we have

$$T = \frac{2\cos\phi}{1+\cos\phi}, \qquad R = \frac{1-\cos\phi}{1+\cos\phi} \tag{43}$$

which show that at normal incidence the transmission and reflection probabilities are unity and zero, respectively. Also note that in the case of no electrostatic potential ($V_0 = 0$) we get

$$T = \frac{2q_x}{k_x + q_x}, \qquad R = \frac{k_x - q_x}{k_x + q_x} \tag{44}$$

which is exactly the same result obtained in [13], showing that T always remains smaller than one, as there is no way for k and q to be equal.

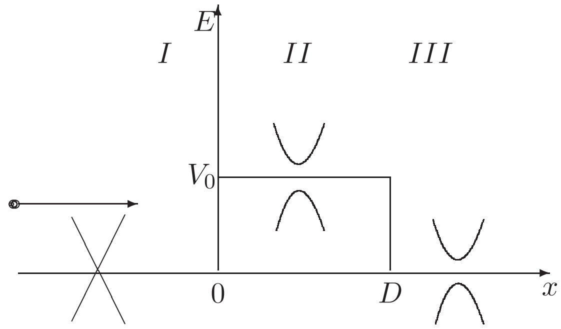

Figure 3. A barrier of height V_0 and width D under which massless electrons acquire a finite mass.

Before we proceed to the case of the potential barrier and consequences that the π phase change might have on probability, we attract the reader's attention to the fact that this phase change is equivalent to the rotation of momentum vector $\mathbf{q}$ by 180°, meaning that the direction of the momentum and group velocity is antiparallel which itself leads to the negative refraction in graphene reported by Cheianov [14].

4. A special n–p–n junction

In this section we suggest a structure, which is schematically shown in figure 3, for an n–p–n junction that would never be transparent even at resonance conditions. This n–p–n junction is such that massless electrons can go through a region of finite gap where there is an electrostatic potential of height V_0. Here we consider a massless electron approaching this type of barrier with energy $E < V_0$. Considering the normal incidence, the electron wavefunction then follows the time independent one-dimensional (1D) Dirac-like equation:

$$(v_{\rm F}\sigma^x p + V(x))\psi = E\psi,$$
$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < D \\ 0 & x > D. \end{cases} \tag{45}$$

The line $x = 0$ separates the regions of gapped and gapless graphene. Hence electrons are massless for $x < 0$ and acquire a finite mass equal to $\Delta/2v_{\rm F}^2$ for $x > 0$. Now assuming the electron is propagating from the left and considering the π phase change of the transmitted wavefunction in the momentum space, we obtain three solutions—one before the barrier in region I

$$\psi_{\rm I} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}{\rm e}^{{\rm i}k'_x x} + \frac{r}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}{\rm e}^{-{\rm i}k'_x x}, \tag{46}$$

and one under the electrostatic potential in region II

$$\psi_{\rm II} = \frac{a}{\sqrt{2}}\begin{pmatrix}\beta\\\eta\end{pmatrix}{\rm e}^{{\rm i}q_x x} + \frac{b}{\sqrt{2}}\begin{pmatrix}\beta\\-\eta\end{pmatrix}{\rm e}^{-{\rm i}q_x x}, \tag{47}$$

and finally one after the barrier in region III

$$\psi_{\rm III} = \frac{t}{\sqrt{2}}\begin{pmatrix}\alpha\\\gamma\end{pmatrix}{\rm e}^{{\rm i}k_x x}. \tag{48}$$

Both incoming and the reflected part of the transmitted wavefunctions are associated with the positive values for the x-component of the momentum vector, whereas the transmitted parts of ψ_{II} like the reflected parts of ψ_{I} are associated with negative values for x-components of $\mathbf{q}$ and $\mathbf{k}$, respectively. Now the momentum in the different regions I, II and III are, respectively, given by

$$k'_x = \frac{E}{v_{\mathrm{F}}}, \tag{49}$$

$$q_x = -\sqrt{\frac{(E - V_0)^2 - \Delta^2}{v_{\mathrm{F}}^2}}, \tag{50}$$

$$k_x = \sqrt{\frac{E^2 - \Delta^2}{v_{\mathrm{F}}^2}}. \tag{51}$$

At this point, by imposing the continuity conditions of waves functions, we obtain the following set of equations:

$$1 + r = \beta(a + b), \tag{52}$$

$$1 - r = \eta(a - b), \tag{53}$$

$$a\beta \mathrm{e}^{\mathrm{i}q_x D} + b\beta \mathrm{e}^{-\mathrm{i}q_x D} = t\alpha \mathrm{e}^{\mathrm{i}k_x D}, \tag{54}$$

$$a\eta \mathrm{e}^{\mathrm{i}q_x D} - b\eta \mathrm{e}^{-\mathrm{i}q_x D} = t\gamma \mathrm{e}^{\mathrm{i}k_x D} \tag{55}$$

which solving them with respect to t gives the transmission amplitude as

$$t = \frac{4\mathrm{e}^{-\mathrm{i}k_x D}}{u\mathrm{e}^{\mathrm{i}q_x D} - v\mathrm{e}^{-\mathrm{i}q_x D}}, \tag{56}$$

where we have defined

$$u = (\beta - \eta)\left(\frac{\alpha}{\beta} - \frac{\gamma}{\eta}\right), \qquad v = -(\beta + \eta)\left(\frac{\alpha}{\beta} + \frac{\gamma}{\eta}\right), \tag{57}$$

for the ease of calculations of $|t|^2$ which is given by

$$|t|^2 = \frac{16}{(u - v)^2 + 4uv\sin^2(q_x D)}. \tag{58}$$

Here, one has to use the equations of previous sections to obtain the probability. Thus, with

$$j_x^{in} = 1, \qquad j_x^r = -|r|^2, \qquad j_x^t = \alpha\gamma|t|^2, \tag{59}$$

the transmission probability, using the relation ($R + T = 1$), is found to be as follows:

$$T = \alpha\gamma|t|^2. \tag{60}$$

Therefore probability for a massless electron to pass through the barrier is given by

$$T = \frac{16\alpha\gamma}{(u - v)^2 + 4uv\sin^2(q_x D)} \tag{61}$$

where

$$(u - v)^2 = 4(\alpha + \gamma)^2 = 8\frac{E + \sqrt{E^2 - \Delta^2}}{E}. \tag{62}$$

Now we are able to write down the expression for transmission as

$$T = \frac{2\sqrt{E^2 - \Delta^2}}{E + \sqrt{E^2 - \Delta^2} + 2\frac{\Delta^2(E - \lambda\lambda'|V_0 - E|)}{v_{\mathrm{F}}^2 q^2}\sin^2(q_x D)}. \tag{63}$$

It is evident that probability depends on $\lambda' = \pm 1$, contrary to the result (42). Interestingly, we see that the confinement of the electrostatic potential to a region with width D, leads to dependence of the probability on $\lambda' = \pm 1$, unlike the step case (see section 3). At this point, we emphasize that the solution (63) for the probability, as one can show, holds for the case of $E > V_0$ as well. This solution shows that for the values of q_x satisfying the relation:

$$q_x D = n\pi, \tag{64}$$

with n an integer, and

$$\alpha\gamma = \frac{\sqrt{E^2 - \Delta^2}}{E} = \frac{k_x}{k'_x}, \tag{65}$$

we have:

$$T = \frac{16\alpha\gamma}{(u - v)^2} = \frac{2k_x}{k_x + k'_x}. \tag{66}$$

As one can see when the resonance condition is satisfied, the barrier is not completely transparent. This result may be of interest in applications for which the resonance tunneling is unwanted. We also see that the transmission in this case is independent of the electrostatic potential.

4.1. Tunneling through n–p–n junctions

Now we turn our attention to the case of the tunneling of an electron with energy E across a 2D potential barrier with height V_0 and width D in pure graphene. Therefore, the wavefunctions in the three regions can be written as

$$\psi_{\mathrm{I}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \lambda \mathrm{e}^{\mathrm{i}\phi} \end{pmatrix} \mathrm{e}^{\mathrm{i}(k_x x + k_y y)} + \frac{r}{\sqrt{2}}\begin{pmatrix} 1 \\ \lambda \mathrm{e}^{\mathrm{i}(\pi - \phi)} \end{pmatrix} \mathrm{e}^{\mathrm{i}(-k_x x + k_y y)}, \tag{67}$$

$$\psi_{\mathrm{II}} = \frac{a}{\sqrt{2}}\begin{pmatrix} 1 \\ \lambda' \mathrm{e}^{\mathrm{i}\theta_t} \end{pmatrix} \mathrm{e}^{\mathrm{i}(q_x x + k_y y)} + \frac{b}{\sqrt{2}}\begin{pmatrix} 1 \\ \lambda' \mathrm{e}^{\mathrm{i}(\pi - \theta_t)} \end{pmatrix} \mathrm{e}^{-\mathrm{i}(q_x x + k_y y)}, \tag{68}$$

$$\psi_{\mathrm{III}} = \frac{t}{\sqrt{2}}\begin{pmatrix} 1 \\ \lambda \mathrm{e}^{\mathrm{i}\phi} \end{pmatrix} \mathrm{e}^{\mathrm{i}(k_x x + k_y y)}. \tag{69}$$

In the next step by imposing the continuity condition of the wavefunctions at the boundaries ($x = 0$ and D), we obtain the following system of equations:

$$1 + r = a + b \tag{70}$$

$$\lambda \mathrm{e}^{\mathrm{i}\phi} - \lambda r \mathrm{e}^{-\mathrm{i}\phi} = \lambda' a \mathrm{e}^{\mathrm{i}\theta_t} - \lambda' b \mathrm{e}^{-\mathrm{i}\theta_t} \tag{71}$$

$$a\mathrm{e}^{\mathrm{i}q_x D} + b\mathrm{e}^{-\mathrm{i}q_x D} = t\mathrm{e}^{\mathrm{i}k_x D} \tag{72}$$

$$\lambda' a \mathrm{e}^{\mathrm{i}\theta_t + \mathrm{i}q_x D} - \lambda' b \mathrm{e}^{-\mathrm{i}\theta_t - \mathrm{i}q_x D} = \lambda t \mathrm{e}^{\mathrm{i}\phi + \mathrm{i}k_x D} \tag{73}$$

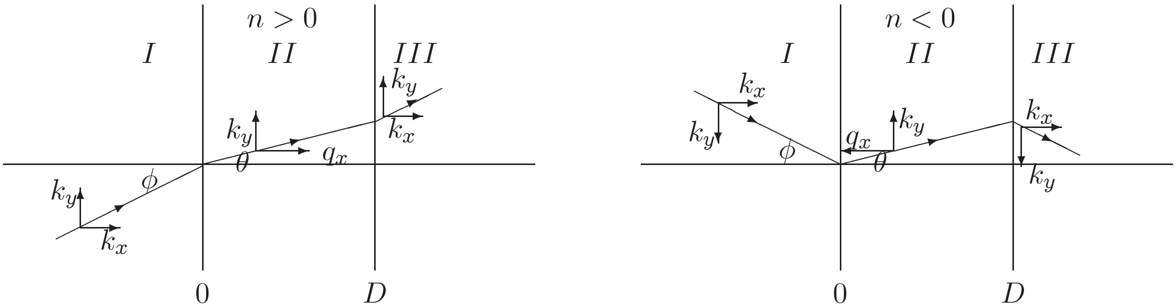

Figure 4. Two electrons incident upon a potential barrier with the same angles of incidence ϕ and the same magnitude for $|\mathbf{q}|$ ($|V_0 - E|$). Left (right): $E > V_0$ ($E < V_0$) and therefore $n > 0$ ($n < 0$).

from which one can calculate the transmission as follows:

$$T(\phi) = \frac{\cos^2\phi\cos^2\theta_t}{(\cos\phi\cos\theta_t\cos(q_x D))^2 + \sin^2(q_x D)(1 - \lambda\lambda'\sin\phi\sin\theta_t)^2} \tag{74}$$

which is the transmission for massless Dirac fermions in gapless graphene and, as we will show in what follows, is not exactly the same result as the one in [12]. The point is that in the case of $E < V_0$, since $\lambda\lambda' = -1$ and $\theta_t = \theta + \pi$ we have

$$T(\phi) = \frac{\cos^2\phi\cos^2\theta}{(\cos\phi\cos\theta\cos(q_x D))^2 + \sin^2(q_x D)(1 - \sin\phi\sin\theta)^2} \tag{75}$$

and also in the case of $E > V_0$, as $\lambda\lambda' = 1$ and consequently $\theta_t = \theta$, the above result holds as well. So, we see that in [12] and [11][6] the angle that momentum vector $\mathbf{q}$ makes relative to the normal incidence has been confused with the propagation (refraction) angle of the wavepacket, i.e. the angle that the associated group velocity makes with respect to the normal incidence. Note that on page 8 of [12] (i) the minus sign for q_x is neglected and (ii) the authors claim that, in the limit $\phi = 0$, $\theta = 0$ while in this limit depending on $\lambda' = \mathrm{sgn}(V_0 - E)$, θ can be either zero and π. However, as we showed above for equal values of q_x and either cases of $\lambda' = 1$ and -1, we get the same results for T, irrespective of whether the incident electron's energy is higher or smaller than the height of the electrostatic barrier. For further illustration, consider the situation depicted in figure 4. We see that for a certain incident angle, those electrons for which the value of $|V_0 - E|$ (and therefore the group velocity) is the same, penetrate the barrier with the same probability regardless of whether the sign of the refractive index, n, is positive or negative. To be more specific, as depicted in figure 4 (for the sake of a simplified illustration the reflected parts of waves are not shown), in spite of the fact that for both cases the associated electron waves travel the same path in the region of the electrostatic potential and also the velocity of the quasi-particle, whether it is an electron or a hole, is the same, the expression for T gives the same results, while one would not arrive at the same values

[6] The term $ss'\sin\theta$ in equation (3) gives different values for both cases of $s' = \pm 1$. This is because in this paper the negative sign for q_x has not been considered and therefore $\theta = \tan^{-1}(k_y/q_x)$ indicates the propagation angle and falls between $[0, \pi/2]$.

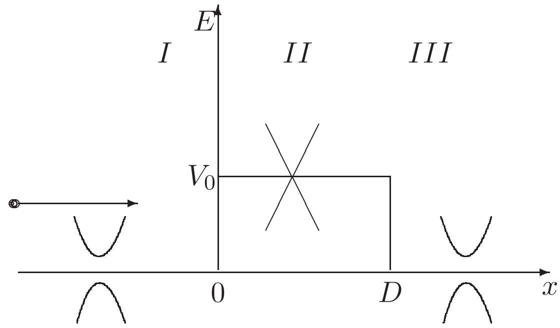

Figure 5. A barrier of height V_0 and width D in which the quasi-particles lose their mass.

for T if transmission depends on the band index in the region of the electrostatic potential. However, for a heterostructure for which the region of the electrostatic potential exhibits no gap and instead the gaps are in regions I and III (see figure 5), one can show that the transmission probability is given by the following expression:

$$T(\phi) = \frac{\cos^2\phi\cos^2\theta}{(\cos\phi\cos\theta\cos(q_x D))^2 + \sin^2(q_x D)(\frac{1}{\alpha\gamma} - \sin\phi\sin\theta)^2}, \tag{76}$$

from which it is clear that in the limit of $\phi = 0$, probability is given by:

$$T(0) = \frac{1}{1 + [(1 - \alpha^2\gamma^2)/\alpha^2\gamma^2]\sin^2(q_x D)}. \tag{77}$$

The above expression explicitly shows that T is independent of the band index. Also note that in the limit of no potential we get for $T(0)$

$$T(0) = \frac{1}{1 + [\Delta^2/k_x^2]\sin^2(q_x D)}. \tag{78}$$

Now considering a barrier for which the width of the electrostatic potential and the width of the region of the finite gap are the same so that the linear spectrum is restricted to regions I and III, one can evaluate the transmission probability as follows:

$$T(\phi) = \frac{\cos^2\phi\cos^2\theta}{(\cos\phi\cos\theta\cos(q_x D))^2 + \sin^2(q_x D)(\frac{1}{\eta\beta} - \sin\phi\sin\theta)^2} \tag{79}$$

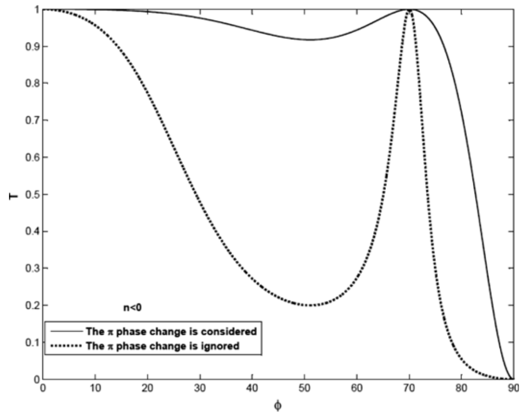

Figure 6. Transmission as a function of ϕ for a barrier of width 50 nm corresponding to the two approaches discussed in this paper.

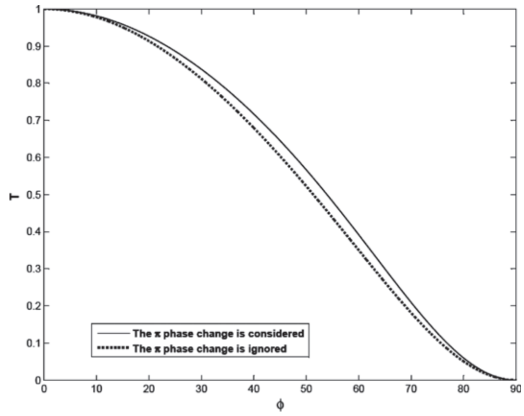

Figure 7. Transmission through pure graphene for a massless electron of $E = 85$ meV and $V_0 = 2000$ based on the two approaches.

which shows that T is again independent of the band index, i.e. the sign of λ'.[7] We see that for an electron approaching perpendicularly to the barrier and in the limit $V_0 \to 0$, transmission is given by

$$T(0) = \frac{1}{1 + [\Delta^2/q_x^2]\sin^2(q_x D)} \tag{80}$$

which is the same result reported in [13].

Note that both equation (74) and that reported in [12], in the case of $\phi = 0$, give $T = 1$, no matter whether the energy of the massless incident electron is higher or lower than V_0 and therefore both results show that $T(0)$ is independent of the band index. Thus, for different angles of incidence, since we have the translational symmetry along the y-direction, one expects that any 2D solution for T would be independent of the band index as well and, as we showed, this is only possible when one considers the π phase change of the transmitted wavefunction (so that the direction of $\mathbf{q}$ differs by 180° relative to the direction of the group velocity) in the case of $E < V_0$. Hence, interestingly, we see that not only by considering the π phase change, one would not arrive at the negative values for transmission into a potential step, but it gives a more reasonable result for the transmission probability corresponding to tunneling of massless electrons in pure graphene through a potential barrier as well. This is important because for computing the conductivity, one can use the Büttiker formula [18]:

$$G = G_0 \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} T(\phi)\cos(\phi)\,\mathrm{d}\phi, \tag{81}$$

where $G_0 = e^2 m v_F w/\hbar^2$, with w the width of the graphene nanoribbon along the y-axis. As is evident from the above equation, in order to obtain the conductivity of the system, it is necessary to take the integral of $T(\phi)$ over all the angles of incidence. Therefore, we see that it is essential to have an expression that gives the correct results corresponding to all the possible values of ϕ.

[7] Note that here θ shows the propagation angle.

5. Numerical results and discussion

In this section, we evaluate the electronic transmission into p–n and n–p–n junctions of graphene and show the results as a function of the angle of incidence, $\phi > 0$ (since for all cases we have $T(\phi) = T(-\phi)$). Here, we consider some cases for which $E < V_0$ in our numerical calculations. Assuming the energy of the incident electron to be 85 meV and the height of the barrier $V_0 = 200$ meV, figure 6 illustrates the behavior of the transmission based on the results reported in [11, 12] and those reported in this paper. We see that, as expected, considerations regarding the π phase change of the wavefunction in the region of the electrostatic potential result in higher values for transmission probability relative to values of transmission for which the π phase change is ignored. However, the angles of incidence for which the resonance condition are satisfied are the same. Interestingly for a very high potential barrier the two expressions give similar values (see figure 7). It is because in the limit $V_0 \to \infty$ we have

$$T(\phi) \simeq \frac{\cos^2(\phi)}{1 - \cos^2(q_x D)\sin^2(\phi)} \tag{82}$$

which reveals that probability like the case $\phi = 0$ is independent of the band index, $\lambda' = \pm 1$, irrespective of whether the π phase change is considered or not.

Now we turn our attention to a p–n junction of gapped graphene and consider the more general case, i.e. two different values for induced gaps $2\Delta_{\mathrm{I}} = 40$ and $2\Delta_{\mathrm{II}} = 60$ meV in regions I and II, respectively; the behavior of the electronic transmission is shown in figure 8. In this figure the results for transmission due to the tunneling of a massless electron into a region of finite gap of 60 meV ($\Delta = 30$ meV) are also depicted. We see that, in this case, one arrives at higher values for T. Hence, in the sense of getting higher values for transmission, a p–n junction that is constructed by connecting a piece of pure graphene and a semiconductor could be a better model to give higher values for the probability.

Finally we evaluated the probability of tunneling into an n–p–n junction with $\Delta = 15$ meV and width of 78 nm as a

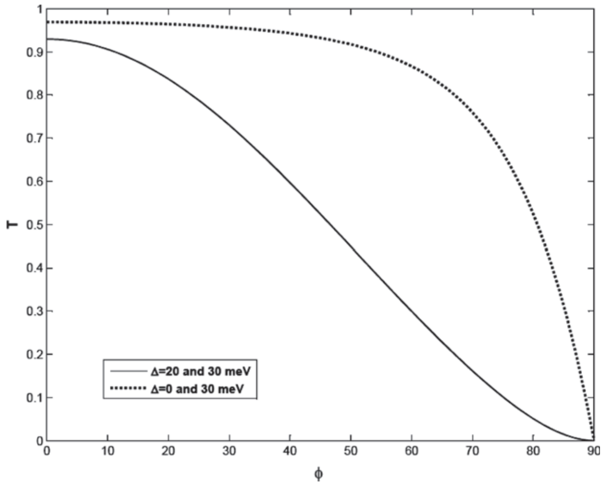

Figure 8. Transmission as a function of ϕ through n–p junctions for two different values of Δ.

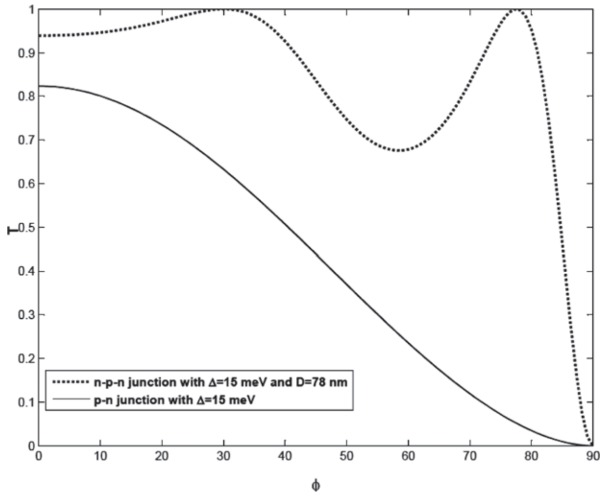

Figure 9. Transmission as a function of ϕ through completely gapped n–p–n and p–n junctions.

function of ϕ. The results are depicted in figure 9. We also evaluated T for a p–n junction with $\Delta = 15$ meV as a function of ϕ. It is seen that there are no resonances for the case of the p–n junction.

6. Conclusion

In this work, first by obtaining the exact expression for the transmission and reflection probabilities of charge carriers in a p–n junction of gapped graphene, we showed that the probability for carriers to penetrate the p–n junction depends on the sign of the refractive index n (graphene meets negative refractive index when the height of the electrostatic potential exceeds the energy of the incident electrons [14]). We then studied the tunneling of a massless electron of energy E, transmitted into a p–n junction of graphene, which allowed the electron to acquire an effective mass of $\frac{\Delta}{v_F^2}$ and found that, unlike the latter case, the transmission probability is independent of the band index (or equivalently the sign of the refractive index) in the region of the electrostatic potential. We also showed that simply by considering the appropriate transmitted wavefunction associated to an electron propagating with energy $E < V_0$ (with V_0 the height of the potential step), the transmission and the reflection probability both turn out to be positive and smaller than unity instead of being negative and therefore higher than the unity reflection coefficient reported in some papers [19–21]. The correct transmitted wavefunction was revealed by consideration of the opposite directions that the group velocity and the momentum vector $\mathbf{q}$ of an electron with energy $E < V_0$ must have under the electrostatic potential. In other words, the transmitted wavefunction in momentum space in this case undergoes a π phase change when passing through the region of the electrostatic potential, meaning that the momentum vector rotates by 180° relative to the direction in which the transmitted wavepacket propagates in this region. We then suggested a model for an n–p–n junction that even at the resonance condition, $q_x D = n\pi$, would not be completely transparent. This model could be of interest in applications for which the resonance tunneling is considered an unwanted phenomenon.

In section 4.1 we studied the transmission of an incident electron across a heterojunction of width D (equivalent to a p–n–p junction of a graphene nano-transistor) under which the electron acquired a finite mass, due to the presence of a gap of 2Δ in the spectrum of graphene, and showed that the existence of the linear spectrum in some spatial regions leads to independence of the probability from the band index. This may be useful for detecting the regions in which graphene exhibits a linear dispersion relation. In this subsection we also, by taking account of the appropriate wavefunctions of an electron with energy $E < V_0$, found that for both cases $\lambda' = 1$ and -1 (with the same magnitude for q_x) one arrives at the same results for transmission probability, contrary to the result reported for T in [12] (note that in [11] the reflection coefficient has been evaluated).

Here, we want to emphasize that our aim is not to indicate that a few incorrect results have been found in some papers. What really matters is that confusing the angle of the propagation of the wavepacket[8] with the angle that the momentum vector makes with respect to the x-axis, not only gives negative values for transmission probability corresponding to the Klein tunneling of charge carriers into a step potential, but, as we showed in section 4.1, leads to a counterintuitive result for tunneling through a potential barrier. This result could be considered as theoretical evidence that the same procedure which leads to a higher than unity reflection coefficient for a potential step, also gives counterintuitive results for a barrier. It should be noted that, up to now, all the contradictions reported about the Klein paradox have been associated with the potential steps [22] and not the barrier. Based on the pair production theory, the pair annihilation at one of the discontinuities of the potential barrier is considered to account for the positive and less than unity values for T and R, respectively [21].

[8] The angle that group velocity makes relative to normal incidence.

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