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Electronic Tunneling in Graphene

Dariusz Jahani

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1. Introduction

In this chapter the transmission of massless and massive Dirac fermions across two-dimensional p-n and n-p-n junctions of graphene which are high enough so that they correspond to 2D potential steps and square barriers, respectively is investigated. It is shown that tunneling without exponential damping occurs when an relativistic particle is incident on a very high barrier. Such an effect has been described by Oskar Klein in 1929 [1] (for an historical review on Klein paradox see [2]). He showed that in the limit of a high enough electrostatic potential barrier, it becomes transparent and both reflection and transmission probability remains smaller than one [3]. However, some later authors claimed that the reflection amplitude at the step barrier exceeds unity [4,5], implying that transmission probability takes the negative values.

Throughout this chapter, these negative transmission and higher-than-unity reflection probability is referred to as the Klein paradox and not to the transparency of the barrier in the limit $V_0 \rightarrow \infty$ (V_0 is height of the barrier). However, by considering the massless electrons tunneling through a potential step which can correspond to a p-n junction of graphene, as the main aim in the first section, it is clear that the transmission and reflection probability both are positive and the Klein paradox is not then a paradox at all. Thus, one really doesn't need to associate the particle-antiparticle pair creation, which is commonly regarded as an explanation of particle tunneling in the Klein energy interval, to Klein paradox. In fact it will be revealed that the Klein paradox arises because of not considering a π phase change of the transmitted wave function of momentum-space which occurs when the energy of the incident electron is smaller than the height of the electrostatic potential step. In the other words, one arrives at negative values for transmission probability merely because of confusing the direction of group velocity with the propagation direction of particle's wave function or equivalently- from a two-dimensional point of view- the propagation angle with the angle that momentum vector under the electrostatic potential step makes with the normal incidence. Then our attentions turn to the tunneling of massless electrons into a barrier with

the height V_0 and width D . It will be found that the probability for an electron (approaching perpendicularly) to penetrate the barrier is equal to one, independent of V_0 and D . Although this result is very interesting from the point of view of fundamental research, its presence in graphene is unwanted when it comes to applications of graphene to nano-electronics because the pinch-off of the field effect transistors may be very ineffective. One way to overcome these difficulties is by generating a gap in the graphene spectrum. From the point of view of Dirac fermions this is equivalent to the appearing of a mass term in relativistic equation which describes the low-energy excitations of graphene, i.e. 2D the massive Dirac equation:

$$H = -iv_F \sigma \cdot \nabla \pm \Delta \sigma^z \quad (1)$$

where Δ is equal to the half of the induced gap in graphene spectrum and it's positive (negative) sign corresponds to the K (K') point. Then the exact expression for T in gapped graphene is evaluated. Although the presence of massless electrons which is an interesting aspect of graphene is ignored, it'll be seen that how it can save us from doing the calculation once more with zero mass on both sides of the barrier, but non-zero mass inside the barrier. This might be a better model for two pieces of graphene connected by a semiconductor barrier (see fig. 6). Another result that show up is that the expression for T in the former case shows a dependence of transmission on the sign of refractive index, n , while in the latter case it will be revealed that T is independent from the sign of n .

From the above discussion and motivated by mass production of graphene, using 2D massive Dirac-like equation, in the next sections, the scattering of Dirac fermions from a special potential step of height V_0 which electrons under it acquire a finite mass, due to the presence of a gap of 2Δ in graphene spectrum is investigated [2], resulting in changing of it's spectrum from the usual linear dispersion to a hyperbolic dispersion and then show that for an electron with energy $E < V_0$ incident on such a potential step, the transmission probability turns out to be smaller than one in normal incident, whereas in the case of $\Delta \rightarrow 0$, this quantity is found to be unity. In graphene, a p-n junction could correspond to such a potential step if it is sharp enough [6-7].

Here it should be noted that for building up such a potential step, finite gaps are needed to be induced in spatial regions in graphene. One of the methods for inducing these 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 C-C distance of graphene [8,9,10]. One other method is to pattern graphene nanoribbons.[11,12]. In this method graphene planes are patterned such that in several areas of the graphene flake narrow nanoribbons may exist. Here, considering the slabs with SiO_2 -BN interfaces, on top of which a graphene flake is deposit, it is then possible to build up some regions in graphene where the 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 present. Considering this possibility, therefore, the tunneling of electrons of energy E through this type of potential step and also an electrostatic barrier of height V_0 which allows quasi-particles to acquire a finite mass in a region of the width D where the dispersion relation of graphene exhibits a parabolic dispersion is investigated. The potential barrier considered here is such that the width of the region of finite mass and the width of the electrostatics barrier is similar. It will be observed that this kind of barrier is not completely transparent for normal incidence contrary to the case of tunneling of massless Dirac fermions in gapless graphene which leads to the total transparency of the barrier

[13,14]. As mentioned it is a real problem for application of graphene into nano-electronics, since for nano-electronics applications of graphene a mass gap in its energy spectrum is needed just like a conventional semiconductor. We also see that, considering the appropriate wave functions in region of electrostatic barrier reveals that transmission is independent of whether the refractive index is negative or positive[15-17]. There is exactly a mistake on this point in the well-known paper "The electronic properties of graphene" [18].

In the end, throughout a numerical approach the consequences that the extra π -shift might have on the transmission probability and conductance in graphene is discussed [19].

2. Quantum tunneling

According to classical physics, a particle of energy E less than the height V_0 of a potential barrier could not penetrate it because the region inside the barrier is classically forbidden, whereas the wave function associated with a free particle must be continuous at the barrier and will show an exponential decay inside it. The wave function must also be continuous on the far side of the barrier, so there is a finite probability that the particle will pass through the barrier(Fig. 1). One important example based on quantum tunnelling is α -radioactivity which was proposed by Gamow [20-22] who found the well-known Gamow formula. The story of this discovery is told by Rosenfeld [23] who was one of the leading nuclear physicist of the twentieth century.

In the following, before proceeding to the case of massless electrons tunneling in graphene, we concern ourselves to evaluation of transmission probability of an electron incident upon a potential barrier with height much higher than the electron's energy.

2.1. Tunneling of an electron with energy lower than the electrostatic potential

For calculating the transmission probability of an electron incident from the left on a potential barrier of height V_0 which is more than the value of energy as indicated in the Figure 1 we consider the following potential:

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < w \\ 0 & x > w \end{cases} \quad (2)$$

For regions I, the solution of Schrodinger's equation will be a combination of incident and reflected plane waves while in region II, depending on the energy, the solution will be either a plane wave or a decaying exponential form.

$$\psi_I = e^{ikx} + re^{-ikx} \quad (3)$$

$$\psi_{II} = ae^{iqx} + be^{-iqx} \quad (4)$$

$$\psi_{III} = te^{ikx} \quad (5)$$

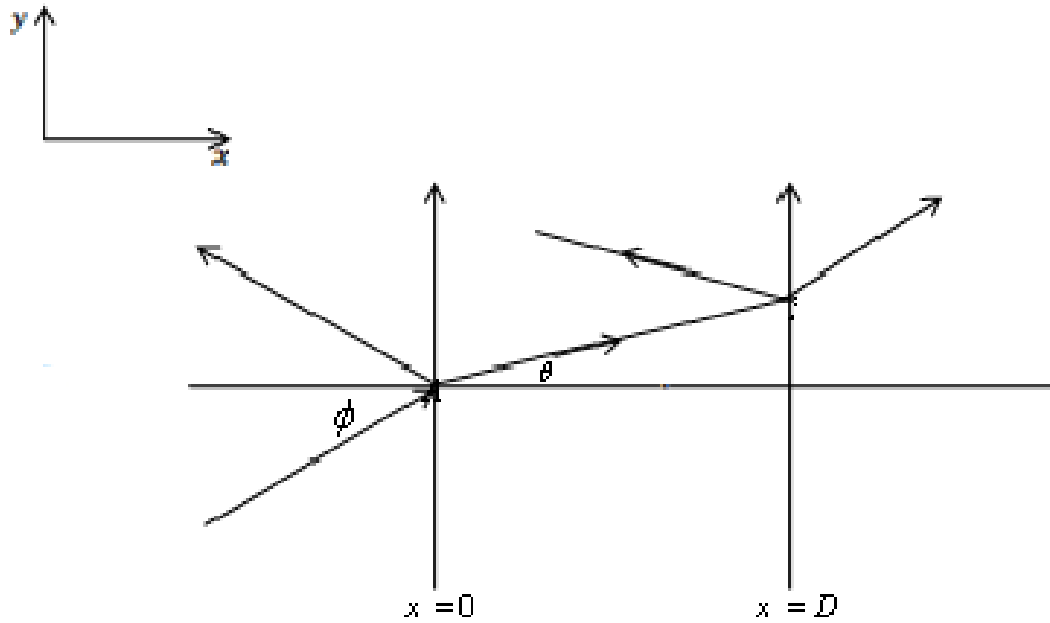


Figure 1. Schematic representation of tunneling in a 2D barrier.

where a, b, r, t are probability coefficients that must be determined from applying the boundary conditions. k and q are the momentum vectors in the regions I and II, respectively:

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad (6)$$

$$q = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}. \quad (7)$$

We know that the wave functions and also their first spatial derivatives must be continuous across the boundaries. Imposing these conditions yields:

$$\begin{cases} 1 + r = a + b \\ ik(1 - r) = iq(a - b) \\ ae^{iqD} + be^{-iqD} = te^{ikD} \\ iq(ae^{iqD} - be^{-iqD}) = kte^{ikD} \end{cases} \quad (8)$$

The transmission amplitude, t is easily obtained:

$$t = \frac{4e^{-ikD}kq}{(q + k)^2e^{-ikD} - (q - k)^2e^{ikD}}, \quad (9)$$

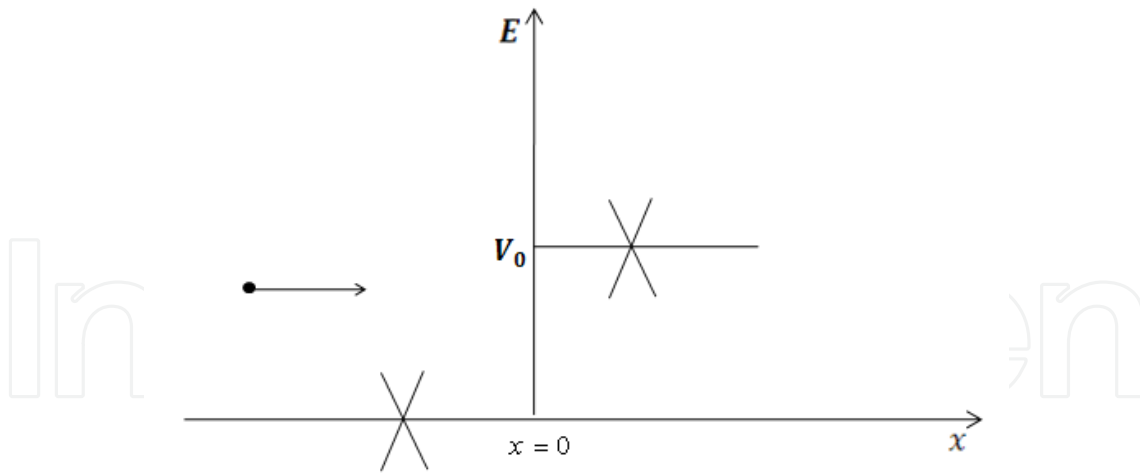


Figure 2. A p-n junction of graphene in which massless electrons incident upon an electrostatic region with no energy gap so that electrons in tunneling process have an effective mass equal to zero.

which from it the transmission probability T can be evaluated as:

$$T = |t|^2 = \frac{16k^2q^2}{(q+k)^2e^{-ikD} - (q-k)^2e^{ikD}}. \quad (10)$$

For energies lower than V_0 , the wave decays exponentially as it passes through the barrier, since in this case q is imaginary. Also note that the perfect transmission happens at $qD = n\pi$ (n an integer). This resonance in transmission occurs physically because of instructive and destructive matching of the transmitted and reflected waves in the potential region. Now that we have got a insight on the quantum tunneling phenomena in non-relativistic limit, the next step is to extent our attentions to the relativistic case.

3. Massless electrons tunneling into potential step

Here, first a p-n junction of graphene which could be realized with a backgate and could correspond to a potential step of hight V_0 on which an massless electron of energy E is incident (see Fig 2) is considered. Two region, therefore, can be considered. The region for which $x < 0$ corresponding to a kinetic energy of E and the region corresponding to a kinetic energy of $E - V_0$. In order to obtain the transmission and reflection amplitudes, we first need to write down the following equation:

$$H = v_F \sigma \cdot p + V(\mathbf{r}), \quad (11)$$

where

$$V(\mathbf{r}) = \begin{cases} V_0 & x > 0 \\ 0 & x < 0 \end{cases} \quad (12)$$

The above Dirac equation for $x > 0$ has the exact solutions which are the same as the free particle solutions except that the energy E can be different from the free particle case by the

addition of the constant potential V_0 . Thus, in the region II, the energy of the Dirac fermions is given by:

$$E = v_F \sqrt{q_x^2 + k_y^2} + V_0, \quad (13)$$

where \mathbf{q} is the momentum in the region of electrostatic potential. The wave functions in the two regions can be written as:

$$\psi_I = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i(\pi - \phi)} \end{pmatrix} e^{i(-k_x x + k_y y)}, \quad (14)$$

and

$$\psi_{II} = \frac{t}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda' e^{i(\theta + \pi)} \end{pmatrix} e^{i(q_x x + k_y y)}, \quad (15)$$

where r and t are reflected and transmitted amplitudes, respectively, $\lambda' = \text{sgn}(E - V_0)$ is the band index of the wave function corresponding to the second region ($x > 0$) and $\phi = \arctan(\frac{k_y}{k_x})$ is the angle of propagation of the incident electron wave and $\theta = \arctan(\frac{k_y}{q_x})$ with

$$q_x = \pm \sqrt{\left[\frac{(V_0 - E)^2}{v_F^2} \right] - k_y^2}, \quad (16)$$

is the angle of the propagation of the transmitted electron wave¹ and not, as it should be, the angle that momentum vector \mathbf{q} makes with the x-axis. The reason will be clear later.

The following set of equations are obtained, if one applies the continuity condition of the wave functions at the interface $x = 0$:

$$1 + r = t \quad (17)$$

$$\lambda e^{i\phi} - r \lambda e^{-i\phi} = \lambda' t e^{i\theta}, \quad (18)$$

which gives the transmission amplitude, t , as follows:

$$t = \frac{2\lambda \cos \phi}{\lambda' e^{i\theta} + \lambda e^{-i\phi}}. \quad (19)$$

Multiplying t by its complex conjugate yields:

$$tt^* = \frac{2 \cos^2 \phi}{1 + \lambda \lambda' \cos(\phi + \theta)}. \quad (20)$$

¹ By this definition θ falls in the range $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$.

Here it should be noted that the transmission probability, T , as we see later, is not simply given by tt^* unlike to the refraction probability, R , which is always equal to rr^* :

$$R = rr^* = \frac{1 - \lambda\lambda' \cos(\phi - \theta)}{1 + \lambda\lambda' \cos(\phi + \theta)}. \quad (21)$$

The reader can easily check that using the relation:

$$R + T = 1. \quad (22)$$

Physically the reason that T is not given by tt^* is because in the conservation law:

$$\nabla \cdot \mathbf{j} + \frac{\partial}{\partial t} |\psi|^2, \quad (23)$$

which gives for the probability current

$$\mathbf{j} = v_F \psi^\dagger \boldsymbol{\sigma} \psi, \quad (24)$$

it is the probability current, $\mathbf{j}(x, y)$, that matters, which is not simply given by probability density $|\psi|^2$. The probability current also contains the velocity which means that if velocity changes between the incoming wave and the transmitted wave, T is not, therefore, given by $|t|^2$, however there is the ratio of the two velocities entering. Here, in order to find the transmission, since the system is translational invariant along the y -direction, we get

$$\nabla \cdot \mathbf{j}(x, y) = 0, \quad (25)$$

which implies that:

$$j_x(x) = \text{constant}. \quad (26)$$

Hence one can write the following relation:

$$j_x^i + j_x^r = j_x^t, \quad (27)$$

where j_x^i , j_x^r and j_x^t denote the incident, reflected and transmission currents, respectively. From this equation it is obvious that:

$$1 = |r|^2 + |t|^2 \frac{\lambda\lambda' \cos \theta}{\sin \phi} \quad (28)$$

One can then obtain the transmission probability from the relation ($R+T=1$) as:

$$T = \frac{2\lambda\lambda' \cos \theta \cos \phi}{1 + \lambda\lambda' \cos(\phi + \theta)}. \quad (29)$$

This equation shows that for an electron of energy $E > V_0$, the probability is positive and also less than unity, whereas for an electron of energy $E < V_0$, as in this case we have $\lambda = 1$ and $\lambda' = \text{sgn}(E - V_0) = -1$, we find that the probability is negative and therefore the reflection probability, R , exceeds unity as it is clear from (21). In fact the assumption of particle-antiparticle (in this case electron-hole) pair production at the interface was considered as an explanation of these higher-than-unity reflection probability and negative transmission and has been so often interpreted as the meaning of the Klein paradox. In particular, throughout this chapter, these features are referred to as the Klein paradox.

Another odd result will be revealed, if we consider the normal incident of electrons upon the interface of the potential step. Assuming an electron propagating with propagation angle $\phi = 0$ on the potential step, we see that both R and T , in this case, become infinite which does not make sense at all because it would imply the existence of a hypothetical current source corresponding to the electron-hole pair creation at interface of the step. In other words no known physical mechanism can be associated to this results.

As it will be clear in what follows the negative T and higher than one reflection probability that equations (29) and (21) imply, arises from the wrong considered direction of the momentum vector, \mathbf{q} , of the wave function in the region II. In fact, in the case of $E < V_0$, momentum and group velocity v_g which is evaluated as:

$$\mathbf{v}_g = \frac{\partial E}{\partial q_x} = \frac{q_x}{E - V_0}, \quad (30)$$

have opposite directions because we assumed that the transmitted electron moves from left to right and therefore v_g must be positive implying that q_x has to assign its negative value, meaning that the direction of momentum in the region II differs by 180 degree from the direction of which the wave packet propagates. In other words in the case of $E < V_0$, the phase of the transmitted wave function in momentum-space undergoes a π change in transmitting from the region I to region II. Thus, the appropriate wave functions in the momentum space, ψ_{II} , is:

$$\psi_{II} = \frac{t}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda' e^{i(\theta+\pi)} \end{pmatrix}, \quad (31)$$

which from them T and R are given by:

$$T = -\frac{2\lambda\lambda' \cos \theta \cos \phi}{1 + \lambda\lambda' \cos(\phi + \theta)}. \quad (32)$$

$$R = \frac{1 + \lambda\lambda' \cos(\phi - \theta)}{1 - \lambda\lambda' \cos(\phi + \theta)}. \quad (33)$$

These expressions now reveal that both transmission and reflection probability are positive and less than unity. It also shows that if electron arrives perpendicularly upon the step, the probability to go through it is one which is related to the well-known "absence of backscattering" [24] and is a consequence of the chirality of the massless Dirac electrons [25]. Notice that in the limit $V_0 \gg E$, since in this case $q_x \rightarrow \infty$ and therefore $\theta \rightarrow 0$, transmission and reflection probability are:

$$T(\phi) = \frac{2 \cos \phi}{1 + \cos \phi}, \quad (34)$$

and

$$R(\phi) = \frac{1 - \cos \phi}{1 + \cos \phi}. \quad (35)$$

As it is clear in the case of normal incident the p-n junction become totally transparent, i.e. $T(0) = 1$.

4. Ultra-relativistic tunneling into a potential barrier

In this section the scattering of massless electrons of energy E by a n-p-n junction of graphene which can correspond to a square barrier if it is sharp enough I address as depicted in figure 3. By writing the wave functions in the three regions as:

$$\psi_I = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i(\pi - \phi)} \end{pmatrix} e^{i(-k_x x + k_y y)}, \quad (36)$$

$$\psi_{II} = \frac{a}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda' e^{i\theta_t} \end{pmatrix} e^{i(q_x x + k_y y)} + \frac{b}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda' e^{i(\pi - \theta_t)} \end{pmatrix} e^{i(q_x x + k_y y)}, \quad (37)$$

$$\psi_{III} = \frac{t}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)}, \quad (38)$$

we'll be able to calculate T only by imposing the continuous condition of wave function at the boundaries and not it's derivative. Note that, in the case of $E < V_0$, $\theta_t = \theta + \pi$ is the angle of momentum vector \mathbf{q} , measured from the x-axis while θ is the angle of propagation of the wave packet and, therefore, shows the angle that group velocity, v_g , makes with the x-axis².

² Notice that if one consider the case $E > V_0$, one then see that $\theta_t = \theta$, implying that momentum and group velocity are parallel.

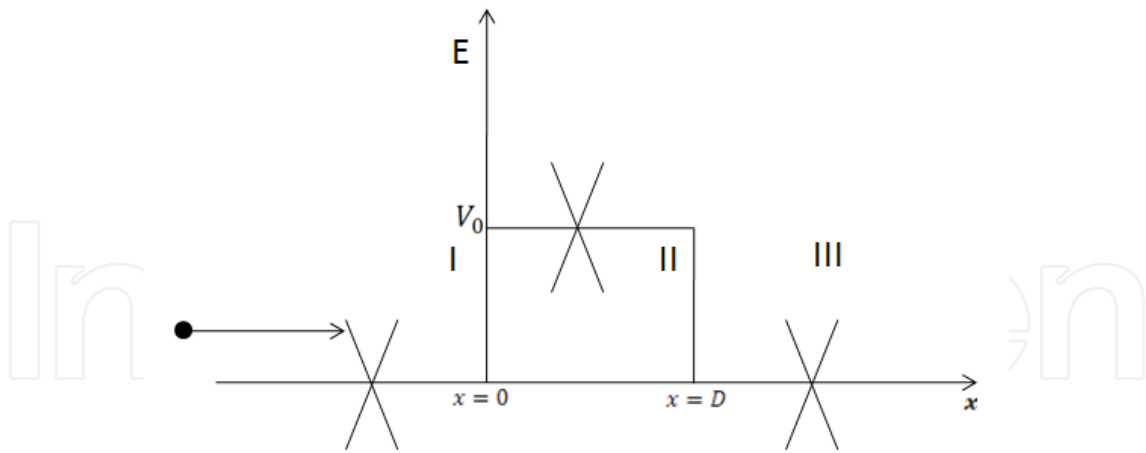


Figure 3. an one dimensional schematic view of a n-p-n junction of gapless graphene. In all three zones the energy bands are linear in momentum and therefore we have massless electrons passing through the barrier.

By applying the continuity conditions of the wave functions at the two discontinuities of the barrier ($x = 0$ and $x = D$), the following set of equations is obtained:

$$1 + r = a + b \quad (39)$$

$$\lambda e^{i\phi} - \lambda r e^{-i\phi} = \lambda' a e^{i\theta_t} - \lambda' b e^{-i\theta_t} \quad (40)$$

$$a e^{iq_x D} + b e^{-iq_x D} = t e^{ik_x D} \quad (41)$$

$$\lambda' a e^{i\theta_t + iq_x D} - \lambda' b e^{-i\theta_t - iq_x D} = \lambda t e^{i\phi + ik_x D}. \quad (42)$$

Here, as previous sections, the transmission amplitude in the first region (incoming wave) is set to 1. For solving the above system of equations with respect to transmission amplitude, t , we first determine a from (41) which turns out to be:

$$a = t e^{-iq_x D + ik_x D} - b e^{-2iq_x D}, \quad (43)$$

and then substituting it in equation (42), b can be evaluated as:

$$b = \frac{t e^{iq_x D + ik_x D} (\lambda' e^{i\theta_t} - \lambda e^{i\phi})}{2\lambda' \cos \theta_t} \quad (44)$$

Now equation (40) by the use of relation (39) could be rewritten as follows:

$$2\lambda \cos \phi = a(\lambda' e^{i\theta_t} + \lambda e^{-i\phi}) - b(\lambda' e^{-i\theta_t} - \lambda e^{-i\phi}). \quad (45)$$

Thus, by plugging a and b into this equation, after some algebraical manipulation t can be determined as:

$$t = -e^{-ik_x D} \frac{4\lambda\lambda' \cos \phi \cos \theta_t}{e^{iq_x D} [2 - 2\lambda\lambda' \cos(\phi - \theta_t)] - e^{-iq_x D} [2 + 2\lambda\lambda' \cos(\phi + \theta_t)]} \quad (46)$$

Up to now, we have only obtained the transmission amplitude and not transmission probability. One can multiply t , by its complex conjugation and get the exact expression for the transmission probability of massless electrons as:

$$T(\phi) = \frac{\cos^2 \phi \cos^2 \theta_t}{(\cos \phi \cos \theta_t \cos(q_x D))^2 + \sin^2(q_x D)(1 - \lambda\lambda' \sin \phi \sin \theta_t)^2} \quad (47)$$

It is evident that $T(\phi) = T(-\phi)$ and for values of $q_x D$ satisfying the relation $q_x D = n\pi$, with n an integer, the barrier becomes totally transparent, as in this case we have $T(\phi) = 1$. Another interesting result will be obtained when we consider the scattering of an electron incident on the barrier with propagation angle $\phi = 0$ ($\phi \rightarrow 0$ leading to $\theta_t \rightarrow 0$ and π for the case of $E > V_0$ and $E < V_0$, respectively) which imply that, no matter what the value of $q_x D$ is, the barrier becomes completely transparent, i.e. $T(0) = 1$. However for applications of graphene in nano-electronic devices such as a graphene-based transistors this transparency of the barrier is unwanted, since the transistor can not be pinched off in this case, however, in the next section by evaluating the transmission probability of a n-p-n junction of graphene which quasi-particles can acquire a finite mass there, it will be clear that transmission is smaller than one and therefore suitable for applications purposes. Turning our attention back to expression (47), it is clear that if one considers the cases $E > V_0$ and $E < V_0$ with the same magnitude for x-component of momentum vector \mathbf{q} , corresponding to same values for $|V_0 - E|$, would arrive at the same results for transmission probability, irrespective of whether the energy of incident electron is higher or smaller than the height of the barrier³. This is a very interesting result because it shows that transmission is independent of the sign of refractive index n of graphene, since for the case of $E < V_0$ group velocity and the momentum vector in the region II have opposite directions and graphene, therefore, meets the negative refractive index. There is a mistake exactly on this point in [18]. In this paper the angle that momentum vector \mathbf{q} makes with the x-axis have been confused with the propagation angle θ . In fact the negative sign of q_x have not been considered there and therefore expression for T which is written there as

$$T(\phi) = \frac{\cos^2 \phi \cos^2 \theta}{(\cos \phi \cos \theta \cos(q_x D))^2 + \sin^2(q_x D)(1 - \lambda\lambda' \sin \phi \sin \theta)^2}, \quad (48)$$

results in different values for probability when $|E - V_0|$ is the same for both cases of $E > V_0$ and $E < V_0$. In other words, the π phase change of the transmitted wave function

³ Because if we assume that energy of incident electron is smaller than height of the barrier, the band index λ' assigns its negative value, meaning that the transmission angle θ_t is $\theta_t = \theta + \pi$ and therefore we get $\sin \theta_t = -\sin \theta$.

in momentum-space in the latter case is not counted in. It is worth noticing that both expressions for normal incident lead to same result $T(0) = 1$.

For a very high potential barrier ($V_0 \rightarrow \infty$), we have $\theta \rightarrow 0, \pi$, and, therefore, we arrive at the following result for T:

$$T(\phi) = \frac{\cos^2 \phi}{\cos^2 \phi \cos^2(q_x D) + \sin^2(q_x D)} = \frac{\cos^2 \phi}{1 - \cos^2(q_x D) \sin^2 \phi}, \quad (49)$$

which reveals that for perpendicular incidence the barrier is again totally transparent.

5. Tunnelling of massive electrons into a p-n junction

In the two previous sections the tunneling of massless Dirac fermions across p-n and n-p-n junctions was covered. In this section the massive electrons tunneling into a two dimensional potential step (n-p junction) of a gapped graphene which shows a hyperbolic energy spectrum unlike to the linear dispersion relation of a gapless graphene is discussed (see Fig. 4). The low energy excitations, therefore, are governed by the two dimensional 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 massive Dirac fermions in gapped graphene so that we'll be able to write down the wave functions in different regions:

$$H = v_F \boldsymbol{\sigma} \cdot \mathbf{p} + \Delta \sigma^z, \quad (50)$$

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

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (51)$$

the $i=x,y,z$, Pauli matrix. Now for obtaining the eigenfunctions one may rewrite the Hamiltonian as:

$$H = \begin{pmatrix} \Delta & v_F |\mathbf{p}| e^{-i\varphi_{\mathbf{p}}} \\ v_F |\mathbf{p}| e^{i\varphi_{\mathbf{p}}} & \Delta \end{pmatrix}, \quad (52)$$

where

$$\varphi_{\mathbf{p}} = \arctan(p_y / p_x). \quad (53)$$

As one can easily see the corresponding eigenvalues are given by:

$$E = \lambda \sqrt{\Delta^2 + v_F^2 \mathbf{P}^2}, \quad (54)$$

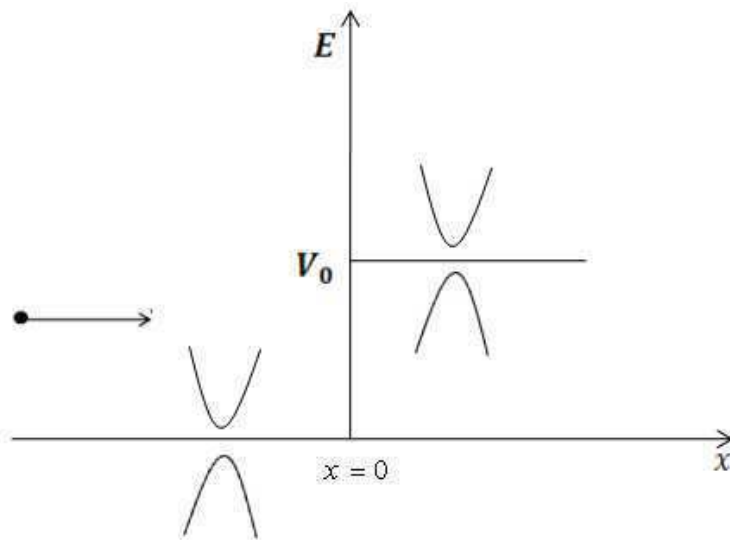


Figure 4. Massive Dirac electron tunneling into a step potential of graphene. As it is clear an opening gap in graphene spectrum makes electrons to acquire an effective mass of $\Delta/2v_F^2$ in both regions

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

$$\psi_{\lambda,\mathbf{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} u_{\lambda} \\ v_{\lambda} \end{pmatrix} e^{i(k_x x + k_y y)}, \quad (55)$$

where we've used units such that $\hbar = 1$. Plugging the above spinors into the corresponding eigenvalue equation then gives:

$$u_{\lambda} = \sqrt{1 + \frac{\lambda \Delta}{\sqrt{\Delta^2 + v_F^2 k^2}}}, \quad v_{\lambda} = \lambda \sqrt{1 - \frac{\lambda \Delta}{\sqrt{\Delta^2 + v_F^2 k^2}}} e^{i\varphi_k}. \quad (56)$$

The wave functions, therefore are given by:

$$\psi_{\lambda,\mathbf{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 + \frac{\lambda \Delta}{\sqrt{\Delta^2 + v_F^2 k^2}}} \\ \lambda \sqrt{1 - \frac{\lambda \Delta}{\sqrt{\Delta^2 + v_F^2 k^2}}} e^{i\varphi_k} \end{pmatrix} e^{i(k_x x + k_y y)}. \quad (57)$$

It is clear that in the limit $\Delta \rightarrow 0$, one arrives at the same eigenfunctions

$$\psi_{\lambda,\mathbf{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i\varphi_k} \end{pmatrix} e^{i(k_x x + k_y y)}, \quad (58)$$

as those of massless Dirac fermions in graphene.

Now that we have found the corresponding eigenfunctions of Hamiltonian (4.52), assuming an electron incident upon a step of height V_0 , we can write the single valley Hamiltonian as:

$$H = v_F \boldsymbol{\sigma} \cdot \mathbf{p} + \Delta \sigma^z + V(\mathbf{r}), \quad (59)$$

where $V(\mathbf{r}) = 0$ for region I ($x < 0$) and for the region II ($x > 0$), massive Dirac fermions feel a electrostatic potential of hight V_0 with the kinetic energy $E - V_0$. The wave functions in the two regions then are:

$$\psi_I = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \\ \gamma \lambda e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \begin{pmatrix} \alpha \\ \gamma \lambda e^{i(\pi - \phi)} \end{pmatrix} e^{i(-k_x x + k_y y)} \quad (60)$$

and

$$\psi_{II} = \frac{t}{\sqrt{2}} \begin{pmatrix} \beta \\ \lambda' \eta e^{i\theta_t} \end{pmatrix} e^{i(q_x x + k_y y)}, \quad (61)$$

where in order to make things more simple, the following abbreviations is introduced:

$$\alpha = \sqrt{1 + \frac{\lambda \Delta}{\sqrt{\Delta^2 + v_F^2 (k_x^2 + k_y^2)}}}, \quad \gamma = \sqrt{1 - \frac{\lambda \Delta}{\sqrt{\Delta^2 + v_F^2 (k_x^2 + k_y^2)}}}, \quad (62)$$

$$\beta = \sqrt{1 + \frac{\lambda' \Delta}{\sqrt{\Delta^2 + v_F^2 (q_x^2 + k_y^2)}}}, \quad \eta = \sqrt{1 - \frac{\lambda' \Delta}{\sqrt{\Delta^2 + v_F^2 (q_x^2 + k_y^2)}}}. \quad (63)$$

Imposing the continuity conditions of ψ_I and ψ_{II} at the interface leads to the following system of equations:

$$\alpha + \alpha r = \beta t, \quad (64)$$

$$\lambda \gamma e^{i\phi} - \lambda \gamma r e^{-i\phi} = \lambda' \eta t e^{i\theta_t}, \quad (65)$$

which solving them with respect to r and t gives

$$r = \frac{\lambda e^{i\phi} - \lambda' \frac{\alpha \eta}{\beta \gamma} e^{i\theta_t}}{\lambda' \frac{\alpha \eta}{\beta \gamma} e^{i\theta_t} + \lambda e^{-i\phi}}, \quad (66)$$

and

$$t = \frac{2\lambda \cos \phi}{\frac{\eta}{\gamma} \lambda' e^{i\theta_t} + \frac{\beta}{\alpha} \lambda e^{-i\phi}}. \quad (67)$$

From (1.66) it is straightforward to show that R is:

$$R = \frac{N_r - 2\lambda\lambda' S_r \cos(\phi - \theta_t)}{N_r + 2\lambda\lambda' S_r \cos(\phi + \theta_t)}, \quad (68)$$

where

$$\begin{aligned} N_r &= \frac{\beta^2 \gamma^2 + \alpha^2 \eta^2}{\beta^2 \gamma^2} \\ &= 2 \frac{E|V_0 - E| - \lambda\lambda' \Delta^2}{E|V_0 - E| - \lambda\lambda' \Delta^2 - \lambda|V_0 - E|\Delta + \lambda' E \Delta} \\ &= 2 \frac{E|V_0 - E| - \lambda\lambda' \Delta^2}{(|V_0 - E| + \lambda' \Delta)(E - \lambda \Delta)} \end{aligned} \quad (69)$$

and

$$\begin{aligned} S_r &= \frac{\alpha \eta}{\beta \gamma} \\ &= \frac{E|V_0 - E| - \lambda\lambda' \Delta^2 + \lambda' E \Delta - \lambda|V_0 - E|\Delta}{E|V_0 - E| - \lambda\lambda' \Delta^2 - \lambda' E \Delta + \lambda|V_0 - E|\Delta} \\ &= \frac{(|V_0 - E| + \lambda' \Delta)(E - \lambda \Delta)}{(|V_0 - E| - \lambda' \Delta)(E + \lambda \Delta)} \end{aligned} \quad (70)$$

In the limit $\Delta \rightarrow 0$ we get the same reflection as that of massless case. In the limit of no electrostatic potential we arrive at the logical result $R = 0$. This is important because we see later that for a special potential step in this limit R is not zero. Now one remaining problem is to calculate the transmission probability. So, considering equation (67) and:

$$j_x^{in} = \lambda \alpha \gamma \cos \phi, \quad j_x^r = -\lambda \alpha \gamma \cos \phi, \quad j_x^t = \lambda' \eta \beta \cos \theta_t \quad (71)$$

T is found to be:

$$\begin{aligned} T &= |t|^2 \frac{\lambda \lambda' \eta \beta \cos \theta_t}{\alpha \gamma \cos \phi} \\ &= \frac{4\lambda \lambda' S_t \cos \phi \cos \theta_t}{N_t + 2S_t \lambda \lambda' \cos(\phi + \theta_t)}, \end{aligned} \quad (72)$$

where the following abbreviations is defined:

$$S_t = \frac{\eta\beta}{\alpha\gamma} = \left[\frac{v_F^2 q^2}{\Delta^2 + v_F^2 q^2} \frac{\Delta^2 + v_F^2 k^2}{v_F^2 k^2} \right]^{\frac{1}{2}}$$

$$= \frac{q}{k} \frac{E}{|V_0 - E|}, \quad (73)$$

and

$$N_t = \frac{\eta^2 \alpha^2 + \beta^2 \gamma^2}{\alpha^2 \gamma^2}$$

$$= 2 \frac{E(E|V_0 - E| - \lambda\lambda'\Delta^2)}{v_F^2 k^2 |V_0 - E|}. \quad (74)$$

At this point one can obtain $T(0)$ as follows:

$$T(0) = 2 \frac{v_F^2 |k_x| |q_x|}{E|V_0 - E| - \lambda\lambda'\Delta^2 + v_F^2 |k_x| |q_x|}. \quad (75)$$

Note that S_t and N_t are positive. It is clear that in the case of $V_0 \rightarrow 0$ and $V_0 \rightarrow \infty$ T is one. Also note that in the limit of $\Delta \rightarrow 0$, as:

$$E|V_0 - E| = v_F^2 |k_x| |q_x|, \quad (76)$$

we see that probability is unity in agreement with result obtained for massless case. Another interesting result that expression for T shows is that probability is not independent of the band index contrary to the a gapless step that led to no independency to band index, λ and λ' .

6. The barrier case

Opening nano-electronic opportunities for graphene requires a mass gap in it's energy spectrum just like a conventional semiconductor. In fact the lack of a bandgap on graphene, can limit graphene's uses in electronics because if there is no gaps in graphene spectrum one can't turn off a graphene-made transistor . In this section, motivated by mass production of graphene, we obtain the exact expression for transmission probability of massive Dirac fermions through a two dimensional potential barrier which can correspond to a n-p-n junction of graphene, and show that contrary to the case of massless Dirac fermions which results in complete transparency of the potential barrier for normal incidence, the probability transmission, T , in this case, apart from some resonance conditions that lead to the total transparency of the barrier, is smaller than one. An interesting result is that in the case of q_x satisfy the relation $q_x D = n\pi$, where n is an integer, we again see that tunneling is easier for a barrier than a potential step, i.e the resonance tunneling is occurred.

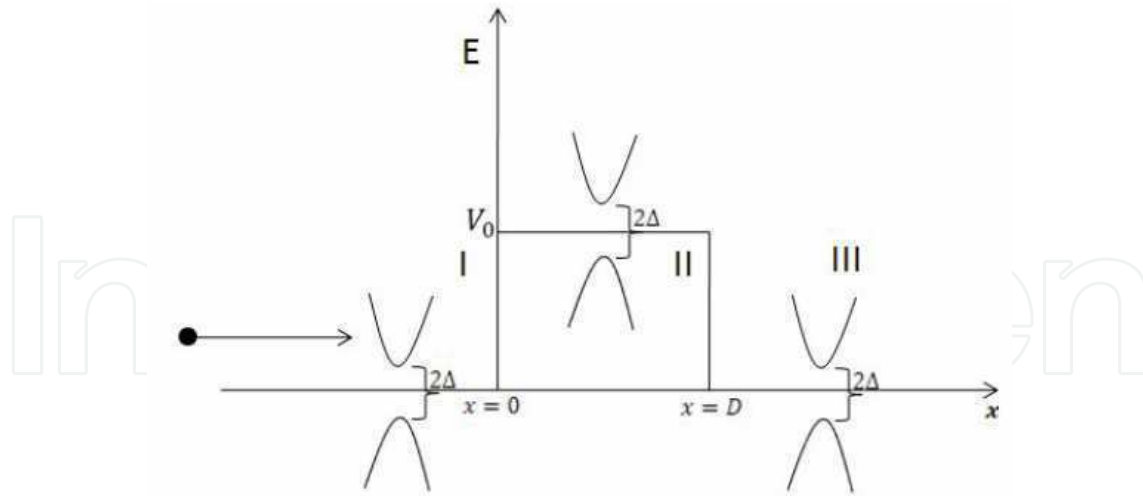


Figure 5. An massive electron of energy E incident on a potential barrier of hight V_0 and thickness of about 50 nm . The opening gap in the all three zones are of the same value and therefore the tunneling phenomenon occurs in a symmetric barrier.

As depicted in the figure 5 there are three regions. The first is for $x < 0$ where the potential is equal to zero. The second region is for $0 < x < D$ where there is a electrostatic potential of hight V_0 and finally, the third region is defined for $x > 0$ and as well as the first region we have $V_0 = 0$. At this point, using equations of previous sections, we are able to write the wave functions in these three different regions in terms of incident and reflected waves. The wave function in region I is then given by:

$$\psi_I = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \\ \lambda \gamma e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \begin{pmatrix} \alpha \\ \lambda \gamma e^{i(\pi - \phi)} \end{pmatrix} e^{i(-k_x x + k_y y)}. \quad (77)$$

In the second region we have:

$$\psi_{II} = \frac{a}{\sqrt{2}} \begin{pmatrix} \beta \\ \lambda' \eta e^{i\theta_t} \end{pmatrix} e^{i(q_x x + k_y y)} + \frac{b}{\sqrt{2}} \begin{pmatrix} \beta \\ \lambda' \eta e^{i(\pi - \theta_t)} \end{pmatrix} e^{i(-q_x x + k_y y)}. \quad (78)$$

In the third region we have only a transmitted wave and therefore the wave function in this region is:

$$\psi_{III} = \frac{t}{\sqrt{2}} \begin{pmatrix} \alpha \\ \lambda \gamma e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} \quad (79)$$

With the continuity of the spinors at the discontinuities, we arrive at the following set of equations:

$$\alpha + \alpha r = \beta a + \beta b \quad (80)$$

$$\lambda \gamma e^{i\phi} - \lambda \gamma r e^{-i\phi} = \eta \lambda' a e^{i\theta_t} - \eta \lambda' b e^{-i\theta_t} \quad (81)$$

$$\beta a e^{iq_x D} + \beta b e^{-iq_x D} = \alpha t e^{ik_x D} \quad (82)$$

$$\eta \lambda' a e^{i\theta_t + iq_x D} - \eta \lambda' b e^{-i\theta_t - iq_x D} = \gamma \lambda t e^{i\phi + ik_x D} \quad (83)$$

Here in order to obtain the transmission T we first solve the above set of equations with respect to transmission amplitude t . So we first need to calculate the coefficients r, a , and b . From (82), a can be written as follows:

$$a = \frac{\alpha}{\beta} t e^{-iq_x D + ik_x D} - b e^{-2iq_x D}, \quad (84)$$

which writing it with respect to transmission amplitude requires to plug b which one can obtain it using the equation (83) as:

$$b = \frac{t e^{iq_x D + ik_x D} (\lambda' \frac{\alpha \eta}{\beta} e^{i\theta_t} - \lambda \gamma e^{i\phi})}{2\lambda' \eta \cos \theta_t}, \quad (85)$$

into the corresponding equation for a . Rewriting (81) by the use of relation $\alpha + \alpha r = \beta a + \beta b$ as:

$$2\lambda \cos \phi = a (\lambda' \frac{\eta}{\gamma} e^{i\theta_t} + \lambda \frac{\beta}{\alpha} e^{-i\phi}) - b (\lambda' \frac{\eta}{\gamma} e^{-i\theta_t} - \lambda \frac{\beta}{\alpha} e^{-i\phi}), \quad (86)$$

and then using the equations (85) and (86), the expression for transmission amplitude yields:

$$t = \frac{-4e^{-ik_x D} \lambda \lambda' \cos \phi \cos \theta}{[e^{iq_x D} (N - 2\lambda \lambda' \cos(\phi - \theta)) - e^{-iq_x D} (N + 2\lambda \lambda' \cos(\phi + \theta))]}, \quad (87)$$

where

$$N = \frac{\eta \alpha}{\beta \gamma} + \frac{\beta \gamma}{\eta \alpha}. \quad (88)$$

It is straightforward to show that:

$$N = 2 \frac{E|V_0 - E| - \lambda \lambda' \Delta^2}{v_F^2 k q}, \quad (89)$$

where

$$E = \sqrt{\Delta^2 + v_F^2 (k_x^2 + k_y^2)} \quad (90)$$

$$|V_0 - E| = \sqrt{\Delta^2 + v_F^2 (q_x^2 + k_y^2)} \quad (91)$$

$$k = \sqrt{k_x^2 + k_y^2} \quad (92)$$

$$q = \sqrt{q_x^2 + k_y^2}. \quad (93)$$

Finally by multiplying t by its complex conjugation, one can obtain the exact expression for the probability transmission of massive electrons, T , as:

$$T(\phi) = \frac{\cos^2 \phi \cos^2 \theta}{(\cos \phi \cos \theta \cos(q_x D))^2 + \sin^2(q_x D) \left(\frac{N}{2} - \lambda \lambda' \sin \phi \sin \theta\right)^2}. \quad (94)$$

It is clear that in the Klein energy interval ($0 < E < V_0$), λ and λ' has opposite signs so that the term $N/2$ in the above expression is bigger than one and, therefore, we see that unlike to the case of massless Dirac fermions which results in complete transparency of the potential barrier for normal incidence, the transmission T for massive quasi-particles in gapped graphene is smaller than one something that is of interest in a graphene transistor. It is obvious that substituting Δ with $-\Delta$ does not change the T , and hence the result for the both Dirac points is the same, as it should be.

Now considering an electron incident on the barrier with propagation angle $\phi = 0$, we know that θ_t becomes 0 (π), depending on the positive (negative) sign of λ' . So in the normal incidence probability reads:

$$T(0) = \frac{2}{2 + (N - 2) \sin^2(q_x D)} \quad (95)$$

Now if the following condition is satisfied:

$$q_x D = n \frac{\pi}{2}, \quad (96)$$

the equation for probability results in:

$$T(0) = \frac{2}{N} = \frac{v_F^2 |k_x| |q_x|}{E |V_0 - E| - \lambda \lambda' \Delta^2} \quad (97)$$

At this point it is so clear that the transmission depends on the sign of $\lambda \lambda' = \pm$. In the other words, this equation for the same values of $|V_0 - E|$, depending on whether E is higher or smaller than V_0 , results in different values for T . The result that have not been revealed before. In the limit $|V_0| \gg |E|$, the exact expression obtained for transmission would be simplified to:

$$T(\phi) \simeq \frac{\cos^2 \phi}{1 - \sin^2 \phi \cos^2(q_x D)} \quad (98)$$

which reveals that in this limit, $T(0)$ is again smaller than one while in the case of $q_x D$ satisfying the condition $q_x D = n\pi$, with n an integer, we still have complete transparency. Furthermore from equations (90) to (93) it is clear that in the limit $\Delta \rightarrow 0$, we get $N/2 = 1$ and, therefore, one arrives at the same expressions for $T(\phi)$ corresponding to the case of massless Dirac fermions i.e. equations (48) and (49). Notice that there is transmission resonances just like other barriers studied earlier. It is important to know that resonances occur when a p-n interface is in series with an n-p interface, forming a p-n-p or n-p-n junction.

7. Transmission into spatial regions of finite mass

In this section the transmission of massless electrons into some regions where the corresponding energy dispersion relation is not linear any more and exhibits a finite gap of Δ is discussed. Thus, the mass of electrons there can be obtained from the relation $mv_F^2 = \Delta$. Starting by looking at a two dimensional square potential step and after obtaining the probability of penetration of step by electrons, transmission of massless electrons into a region of finite mass is investigated and then see how it turns out to be applicable in a transistor composed of two pieces of graphene connected by a conventional semiconductor or linked by a nanotube.

7.1. Tunnelling through a composed p-n junction

In this section 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 is investigated (see Fig. 6). The electrostatic potential under the region of finite mass is:

$$V(\mathbf{r}) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < D \\ 0 & x > D \end{cases} \quad (99)$$

Assuming an electron of energy E , propagating from the left, the wave functions then in the two zones can be written as:

$$\psi_I = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i(\pi - \phi)} \end{pmatrix} e^{i(-k_x x + k_y y)} \quad (100)$$

$$\psi_{II} = \frac{t}{\sqrt{2}} \begin{pmatrix} \beta \\ \lambda' \eta e^{i\theta_t} \end{pmatrix} e^{i(q_x x + k_y y)} \quad (101)$$

where

$$\beta = \sqrt{1 + \frac{\lambda' \Delta}{\sqrt{\Delta^2 + v_F^2 (q_x^2 + k_y^2)}}}, \quad \eta = \sqrt{1 - \frac{\lambda' \Delta}{\sqrt{\Delta^2 + v_F^2 (q_x^2 + k_y^2)}}}, \quad (102)$$

and r and t are reflected and transmitted amplitudes, respectively. Applying the continuity conditions of the wave functions at $x = 0$ yields:

$$1 + r = \beta t \quad (103)$$

$$\lambda e^{i\phi} - r \lambda e^{-i\phi} = \lambda' \eta t e^{i\theta_t} \quad (104)$$

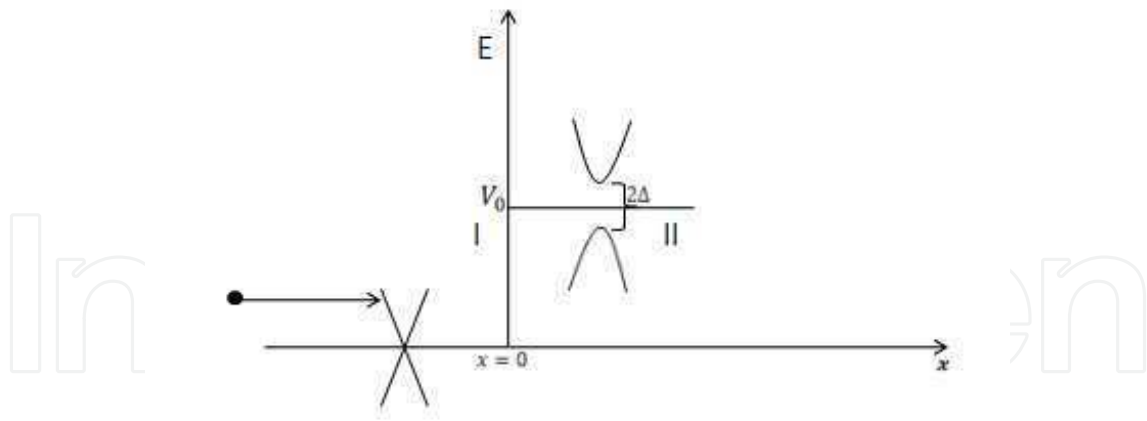


Figure 6. A special potential step of height V_0 and width D which massless electrons of energy E under it acquire a finite mass.

Solving the above equations gives us the following expression for $|t|^2$ and R :

$$|t|^2 = \frac{2 \cos^2 \phi}{1 + \lambda \lambda' \eta \beta \cos(\phi + \theta_t)}, \quad (105)$$

and

$$R = rr^* = \frac{1 - \lambda \lambda' \eta \beta \cos(\phi - \theta_t)}{1 + \lambda \lambda' \eta \beta \cos(\phi + \theta_t)} \quad (106)$$

where

$$\eta \beta = \left[\frac{v_F^2 (q_x^2 + k_y^2)}{v_F^2 (q_x^2 + k_y^2) + \Delta^2} \right]^{\frac{1}{2}} = \frac{v_F q}{|V_0 - E|} \quad (107)$$

For obtaining the transmission probability we need to evaluate the x -component of probability current in two regions. Using equation (24) we get:

$$j_x^{in} = \lambda \cos \phi \quad (108)$$

$$j_x^r = -\lambda \cos \phi |r|^2 \quad (109)$$

$$j_x^t = \lambda' \eta \beta \cos \theta_t |t|^2. \quad (110)$$

Here notice that, using the probability conservation law and the fact that our problem is time independent and invariant along the y -direction, j_x , then has the same values in the two regions. So by the use of relation (27) the following equation come outs:

$$1 - |r|^2 = \frac{\lambda \lambda' \eta \beta \cos \theta_t}{\cos \phi} |t|^2, \quad (111)$$

which once again shows that the probability, T , is not given by $|t|^2$ and instead is:

$$T = \frac{\lambda\lambda'\eta\beta\cos\theta_t}{\cos\phi}|t|^2. \quad (112)$$

The probability, therefore, is given by:

$$T(\phi) = \frac{2\lambda\lambda'\eta\beta\cos\theta_t\cos\phi}{1 + \lambda\lambda'\eta\beta\cos(\phi + \theta_t)}. \quad (113)$$

This result shows that the relation $T(\phi) = T(-\phi)$. Thus, the induced gap in graphene spectrum has nothing to do with relation this relation. We now turn our attention to the case in which an electron is incident perpendicularly upon the step. The probability for this electron to penetrate the step is:

$$\begin{aligned} T(0) &= \frac{2\eta\beta}{1 + \eta\beta} \\ &= \frac{2v_F|q_x|}{|V_0 - E| + v_F|q_x|}, \end{aligned} \quad (114)$$

which shows there is no way for the electron to pass into the step with probability equal to one. However if we consider a potential step which is high enough so that we'll be able to write

$$|V_0 - E| = \sqrt{v_F^2 q_x^2 + \Delta^2} \approx v_F|q_x|, \quad (115)$$

we see the step becomes transparent. So by increasing the potential's height, more electrons can pass through the step. Notice that probability is independent of $\lambda\lambda'$ unlike to the result (72) [19]. Also note that in the limit $\Delta \rightarrow 0$, q_x we can write:

$$v_F|q_x| = |V_0 - E| \quad (116)$$

which immediately gives $T(0)$ as:

$$T(0) = 1, \quad (117)$$

Also note that since for normal incidence we have $E = v_F k_x$, from the equation (114) it is evident that in the case of no electrostatic potential ($V_0 = 0$) we get:

$$T = \frac{2q_x}{k_x + q_x}, \quad R = \frac{k_x - q_x}{k_x + q_x}, \quad (118)$$

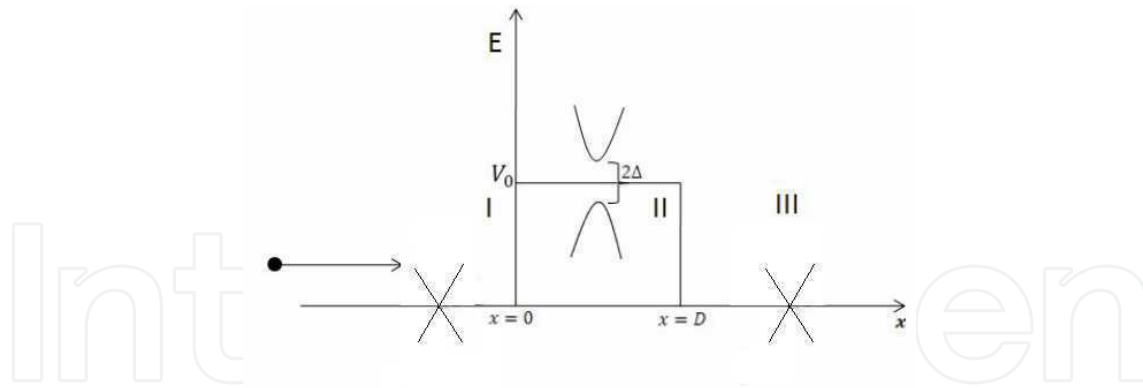


Figure 7. An massless electron of energy E incident (from the left) on a potential barrier of height V_0 and width D , which acquires a finite mass under the electrostatic potential, due to the presence of a gap of 2Δ in the region II. The effective mass of electron in this region is then $m = \Delta/v_F^2$

which shows that probability always remains smaller than one, as there is no way for k and q to be equal⁴. Turning our attention back to equation (113), we see that in the limit $\Delta \rightarrow 0$ one arrives at the following solution for T :

$$T = \frac{2\lambda\lambda' \cos \theta_t \cos \phi}{1 + \lambda\lambda' \cos(\phi + \theta)}, \quad (119)$$

which is just the transmission of massless Dirac fermions through a p-n junction in gapless graphene. This expression now reveals in the limit $V_0 \gg E \approx \Delta$ it can be simplified to the following equation

$$T = \frac{2 \cos \phi}{1 + \cos \phi}, \quad R = \frac{1 - \cos \phi}{1 + \cos \phi} \quad (120)$$

which show that for normal incidence the transmission and reflection probability are unity and zero, respectively.

Here, before proceeding to some numerical calculations in order to depict consequences that the π phase change might have on the probability, I attract the reader's attention to this fact that, the phase change of the wave function in momentum space is equivalent to the rotation of momentum vector, \mathbf{q} by 180 degree, meaning that the direction of momentum and group velocity is antiparallel which itself lead to negative refraction in graphene reported by Cheianov [26,27]. As it clear for imaginary values of q_x an evanescent wave is created in the zone I and a total reflection is observed.

Now, before ending, in order to emphasize on the importance of the π -phase change mentioned earlier some numerical calculations depicting the transmission probability is shown in Fig. 8 which reveal a perceptible difference between result obtained based on considering the π -shift and those obtained if one ignores it. As it is clear for an electron of energy $E = 85 \text{ meV}$, barrier thickness of 100 nm and height of $V_0 = 200 \text{ meV}$ the probability gets smaller values if the extra phase is not considered. This means that considering the

⁴ There is no need to say that when there is no electrostatic potential q_x is positive

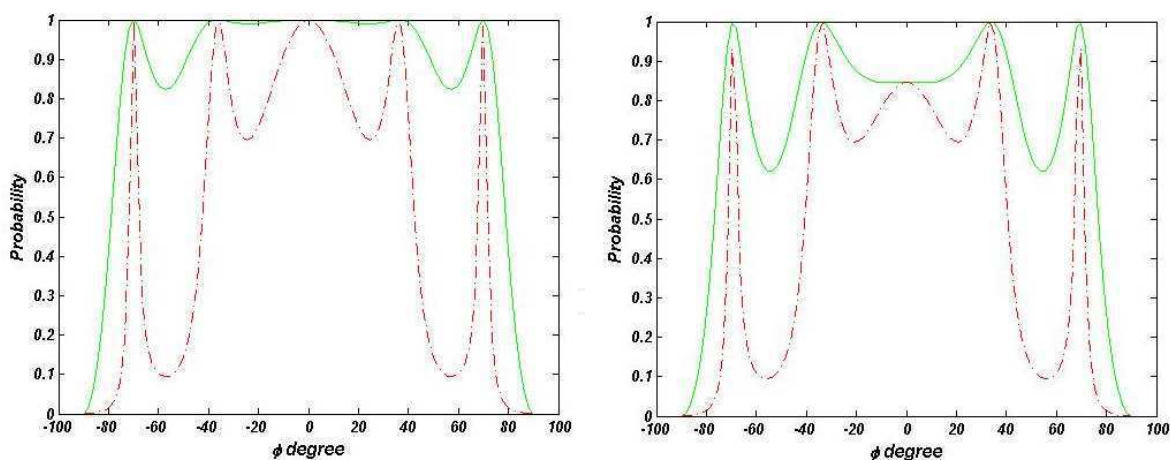


Figure 8. left: Transmission probability as a functions of incident angle for an electron of energy $E = 85\text{meV}$, $D = 100\text{nm}$ and $V_0 = 200\text{meV}$. Right: Transmission in gapped graphene for gap value of 20meV as a functions of incident angle for an electron of energy $E = 85\text{meV}$, $D = 100\text{nm}$ and $V_0 = 200\text{meV}$.

Büttiker formula [28] for conductivity lower conductance is predicted in absence of the extra phase. As it is clear the chance for an electron to penetrate the barrier increases if one chooses the appropriate wave function in the barrier.

The potential application of the theory of extra π phase consideration introduced in the previous sections [19] is that we can have higher conductivity in graphene-based electronic devices and also the results of this work is important in combinations of graphene flakes attached with different energy bands in order to get different kind of n-p-n junctions for different uses. Notice that for nanoelectronic application of graphene the existence of a mass gap in graphene's spectrum is essential because it leads to smaller than one transmission which is of most important for devices such as transistors and therefore the results derived in this work concerning gapped graphene could be applicable in nanoelectronic applications of graphene.

In the end of this chapter I would like to remind that one important result that obtained is that Klein paradox is not a paradox at all. More precisely, it was demonstrated theoretically that the reflection and transmission coefficients of a step barrier are both positive and less than unity, and that the hypothesis of particle-antiparticle pair production at the potential step is not necessary as the experimental evidences confirm this conclusion [29].

Author details

Dariush Jahani

Young Researchers Club, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran

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