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Klein tunneling of massive Dirac fermions in single-layer graphene

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ABSTRACT

For nano-electronics applications of graphene a mass gap in its energy spectrum is needed (like a conventional semiconductor). In this paper, motivated by mass production of graphene, by the use of 2D massive Dirac-like equation we obtain the exact solution for the transmission probability corresponding to the Klein tunneling of massive Dirac fermions through a two-dimensional barrier which can be considered as a n–p–n junction in a graphene nano-transistor, and show that contrary to the case of massless Dirac fermions which results in complete transparency of the barrier for normal incidence, the transmission probability, *T*, in this case, apart from some resonance conditions that lead to the total transparency of the barrier, is smaller than one and also depends on the band index. We then obtain the transmission through a potential barrier in which the massless electrons acquire a finite mass and find that the transmission, in this case, is independent of the band index and cannot reach unity.

1. Introduction

Graphene, a carbon nano-sheet, is a single layer of carbon atoms arranged into a honeycomb lattice. It was isolated for the first time in 2004 [1], and since then has become one of the most studied materials in condensed matter physics. One of the interesting aspects of graphene is that its low energy excitations behave as massless Dirac fermions, instead of massive electrons. These low energy excitations then obey the $(2+1)$–dimensional Dirac equation with the speed of light replaced by the Fermi velocity $v_F \approx 10^6\,\mathrm{m\,s^{-1}}$ [2–5]:

$$-iv_F\boldsymbol{\sigma}.\nabla\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{1}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ and σ_i, with $i = x, y, z$, is the i pauli matrix. One may obtain the corresponding wave functions corresponding to (1) as

$$\psi_{\lambda,\mathbf{k}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \lambda e^{i\varphi_{\mathbf{k}}} \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{2}$$

where $\lambda = \mathrm{sgn}(E)$ is the band index and $\varphi_{\mathbf{k}} = \arctan(k_y/k_x)$. The fact that quasi-particles in graphene are described by the above Dirac-like Hamiltonian is a direct consequence of graphene's crystal symmetry. Its crystal structure consists of two equivalent sublattices A and B [2–4]. Electrons hoping between these two sublattices leads to formation of two energy bands, which touch each other at the edges of the Brillouin zone. These edges consists of six points that two of them are inequivalent and are referred to as Dirac points, say, K and K'. The Hamiltonian (1) leads to the following dispersion relation:

$$E_k = \pm v_F k, \tag{3}$$

which is linear in quasi-particles momentum k, meaning that the velocity of Dirac fermions is independent of their energy. However, resent studies have shown that inducing a finite bandgap in graphene by epitaxially growing it on a substrate [6] is possible and, therefore, its energy dispersion relation is no longer linear in momentum. This generated gaps in graphene energy spectrum which result in a finite mass for its charge carriers, open nano-electronic opportunities for graphene. Thus, instead of Eq. (1), Dirac fermions in gapped graphene are described by the following 2D massive Dirac equation:

$$H = -iv_F\boldsymbol{\sigma}.\nabla \pm \Delta\sigma^z, \tag{4}$$

where Δ is equal to the half of the induced gap in graphene spectrum and positive (negative) sign corresponds to the K (K') point. The corresponding energy eigenvalues of Hamiltonians (4) are given by

$$E_k = \lambda\sqrt{v_F^2k^2 + \Delta^2}. \tag{5}$$

From the above equation it is clear that velocity of Dirac fermions, due to their hyperbolic energy spectrum is no longer constant and, therefore, is energy dependent. Graphene also is a solid-state equivalent of a system of relativistic particles. Thus, the problem

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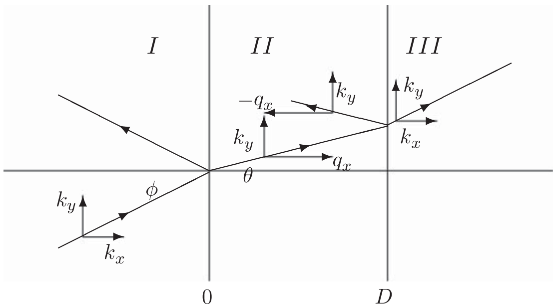

Fig. 1. Square potential barrier with height V_0 and width D.

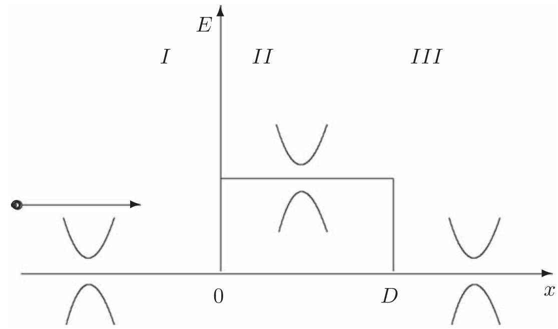

Fig. 2. A massive electron of energy E incident on a potential barrier of hight V_0.

of Klein tunneling of relativistic particles across a potential barrier and the so-called Klein paradox [7,8] which recently has gained more attention can be put to the test. One of the main reasons for this attention is that the potential barrier mentioned here can correspond to a n–p–n junction of graphene if it is high enough and, therefore, it is important to obtain the exact expression for the transmission probability. For massless quasi-particles, this quantity is given by the following expression [8,9]:

$$T=\frac{\cos^2\phi\cos^2\theta}{(\cos\phi\cos\theta\cos q_xD)^2+\sin^2(q_xD)(1-\lambda\lambda'\sin\phi\sin\theta)^2}, \tag{6}$$

where D is width of the barrier and q_x is the component of the momentum along the x-direction in the barrier (see Fig. 1). As it is clear for normal incidence the barrier is completely transparent, i.e. $T(0)=1$. We see that in the case of very high potential barrier, $V0 \gg E$ the above expression takes the following form:

$$T(\phi)\simeq\frac{\cos^2\phi}{1-\cos^2(q_xD)\sin^2(\phi)}, \tag{7}$$

which shows that again there is a perfect transmission at $\phi=0$ and also some resonances which occur when the condition $\cos^2(q_xD)=1$ is satisfied. Now one remaining problem is examining the effect of a induced gap in graphene spectra on the expression for the T, which as was discussed, results in the complete transparency of barrier for normal incidence. This result is unwanted when it comes to application of graphene into nano-electronics. We show that opening a gap in graphene spectrum which results in emerging of massive quasi-particles may be the key to overcome this problem.

In this paper, we first study the tunneling of these particles through a two-dimensional square potential barrier and calculate the exact expression for transmission probability by the use of the two-dimensional massive Dirac equation. Then we turn our attention to the tunneling of a massless electron with energy E into a potential barrier of hight V_0 in which the electron acquires a finite mass of $\Delta/2v_F^2$. This might be a better model in the case connecting two pieces of graphene by a semiconductor barrier.

2. Klein tunneling of massive Dirac fermions through a square potential barrier

In order to calculate transmission probability of massive Dirac fermions (see Fig. 2), we first write down the following two-dimensional Dirac equation corresponding to the K point:

$$H=v_F\boldsymbol{\sigma}\cdot\boldsymbol{p}+\Delta\sigma^z. \tag{8}$$

As in the previous section was mentioned replacing Δ by $-\Delta$ in Eq. (8) gives the Hamiltonian due to the K' point. Then the wave function corresponding to the Hamiltonian (8) by taking $\hbar\equiv1$, follows to be

$$\psi_{\lambda,\mathbf{k}}=\frac{1}{\sqrt2}\begin{pmatrix}\sqrt{1+\dfrac{\lambda\Delta}{\sqrt{\Delta^2+v_F^2k^2}}}\\ \lambda\sqrt{1-\dfrac{\lambda\Delta}{\sqrt{\Delta^2+v_F^2k^2}}}e^{i\varphi_{\mathbf{k}}}\end{pmatrix}e^{i(k_xx+k_yy)}. \tag{9}$$

Note that in the limit $\Delta\to0$ one arrives at the same states

$$\psi_{\lambda,\mathbf{k}}=\frac{1}{\sqrt2}\begin{pmatrix}1\\ \lambda e^{i\varphi_{\mathbf{k}}}\end{pmatrix}e^{i\mathbf{k}.\mathbf{r}}, \tag{10}$$

as those of massless Dirac fermions. Now in order to calculate the transmission probability, T, we write down the single valley Hamiltonian as

$$H=-iv_F\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}+\Delta\sigma^z+V(\mathbf{r}), \tag{11}$$

where $V(\mathbf{r})=0$ for region I ($x<0$) and region III ($x>D$), and for the region II ($D>x>0$) we have $V(\mathbf{r})=V_0$. At this point we are ready to write the wave function in three different region in terms of incident and reflected waves. The wave function in region I is then of the form

$$\psi_I=\frac{1}{\sqrt2}\begin{pmatrix}\alpha\\ \lambda\gamma e^{i\phi}\end{pmatrix}e^{i(k_xx+k_yy)}+\frac{r}{\sqrt2}\begin{pmatrix}\alpha\\ \lambda\gamma e^{i(\pi-\phi)}\end{pmatrix}e^{i(-k_xx+k_yy)}, \tag{12}$$

with $\phi=\arctan(k_y/k_x)$. In the region II we have

$$\psi_{II}=\frac{a}{\sqrt2}\begin{pmatrix}\beta\\ \lambda'\eta e^{i\theta}\end{pmatrix}e^{i(q_xx+k_yy)}+\frac{b}{\sqrt2}\begin{pmatrix}\beta\\ \lambda'\eta e^{i(\pi-\theta)}\end{pmatrix}e^{i(-q_xx+k_yy)}, \tag{13}$$

with $\theta=\arctan(k_y/q_x)$. The x-direction component of the wave-vector in the region II may be written as

$$q_x=\pm\sqrt{((V_0-E)^2-\Delta^2)/v_F^2-k_y^2}, \tag{14}$$

where q_x assigns its negative sign when the energy of incident electron is smaller than hight of potential barrier. In region III we have only a transmitted wave and, therefore, we can write

$$\psi_{III}=\frac{t}{\sqrt2}\begin{pmatrix}\alpha\\ \lambda\gamma e^{i\phi}\end{pmatrix}e^{i(k_xx+k_yy)}, \tag{15}$$

where we have used following abbreviations:

$$\alpha=\sqrt{1+\frac{\lambda\Delta}{\sqrt{\Delta^2+v_F^2k^2}}},\quad \gamma=\sqrt{1-\frac{\lambda\Delta}{\sqrt{\Delta^2+v_F^2k^2}}}, \tag{16}$$

$$\beta=\sqrt{1+\frac{\lambda'\Delta}{\sqrt{\Delta^2+v_F^2(q_x^2+k_y^2)}}},\quad \eta=\sqrt{1-\frac{\lambda'\Delta}{\sqrt{\Delta^2+v_F^2(q_x^2+k_y^2)}}}, \tag{17}$$

where $\lambda'=\mathrm{sgn}(E-V_0)$ is the band index. Now by the use of continuity condition of the wave functions at the boundaries, we arrive at the following set of equations:

$$\alpha+\alpha r=\beta a+\beta b, \tag{18}$$

$$\lambda\gamma e^{i\phi}-\lambda\gamma re^{-i\phi}=\eta\lambda' ae^{i\theta}-\eta\lambda' be^{-i\theta}, \tag{19}$$

$$\beta ae^{iq_xD}+\beta be^{-iq_xD}=\alpha te^{ik_xD}, \tag{20}$$

$$\eta\lambda' ae^{i\theta+iq_xD}-\eta\lambda' be^{-i\theta-iq_xD}=\gamma\lambda te^{i\phi+ik_xD}. \tag{21}$$

Here in order to obtain the transmission T we first solve the above system of equations with respect to transmission amplitude t, which is evaluated as

$$t=\frac{-4e^{-ik_xD}\lambda\lambda'\cos\phi\cos\theta}{[e^{iq_xD}(N-2\lambda\lambda'\cos(\phi-\theta))-e^{-iq_xD}(N+2\lambda\lambda'\cos(\phi+\theta))]}, \tag{22}$$

where

$$N=\frac{\eta\alpha}{\beta\gamma}+\frac{\beta\gamma}{\eta\alpha}. \tag{23}$$

From Eqs. (16) and (17) it is straightforward to show that

$$N=2\frac{E|V_0-E|-\lambda\lambda'\Delta^2}{v_F^2kq}, \tag{24}$$

where

$$E=\sqrt{\Delta^2+v_F^2(k_x^2+k_y^2)}, \tag{25}$$

$$|V_0-E|=\sqrt{\Delta^2+v_F^2(q_x^2+k_y^2)}, \tag{26}$$

$$k=\sqrt{k_x^2+k_y^2}, \tag{27}$$

$$q=\sqrt{q_x^2+k_y^2}. \tag{28}$$

It is by now that one can multiply t, by its complex conjugation and obtain the exact expression for T, the transmission probability of massive electrons as follows:

$$T(\phi)=\frac{\cos^2\phi\cos^2\theta}{(\cos\phi\cos\theta\cos(q_xD))^2+\sin^2(q_xD)\left(\frac{N}{2}-\lambda\lambda'\sin\phi\sin\theta\right)^2}. \tag{29}$$

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 expression (29) 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 which is of interest in a graphene transistor. From relation (24), it is clear that in the limit $\Delta\to 0$, we get $N/2=1$ and, therefore, one arrives at the same expression for $T(\phi)$ corresponding to the case of massless Dirac fermions, i.e. Eq. (6). In the case of normal incident we have

$$T(0)=\frac{2}{2+(N-2)\sin^2(q_xD)}. \tag{30}$$

From this result it is evident that the transmission probability depends on λ', due to appearing of N in this expression.

It is obvious that substituting Δ with $-\Delta$ does not change the result for T, and hence the results for the both Dirac points are the same, as they should be. In the limit $|V_0|\gg|E|$ Eq. (29) becomes

$$T(\phi)\simeq\frac{\cos^2\phi}{1-\sin^2\phi\cos^2(q_xD)}, \tag{31}$$

which reveals that in this limit, $T(0)\simeq 1$.

3. Tunneling of a massless electron through a region of finite gap

Now we turn our attention to the case of the tunneling of an electron with energy E across a two-dimensional potential barrier with the hight V_0 and width D. We suppose that this barrier is such that we have massless electrons on both sides of the barrier, but non-zero mass inside it (see Fig. 3). Thus, in the regions I and III we have massless Dirac fermions, whereas in region II the quasi-particles acquire a finite mass, due to the presence of a finite gap of 2Δ in this region. Therefore, the wave functions in the three regions can be written as

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

$$\psi_{II}=\frac{a}{\sqrt{2}}\begin{pmatrix}\beta\\ \lambda'\eta e^{i\theta}\end{pmatrix}e^{i(q_xx+k_yy)}+\frac{b}{\sqrt{2}}\begin{pmatrix}\beta\\ \lambda'\eta e^{i(\pi-\theta)}\end{pmatrix}e^{i(q_xx+k_yy)}, \tag{33}$$

$$\psi_{III}=\frac{t}{\sqrt{2}}\begin{pmatrix}1\\ \lambda e^{i\phi}\end{pmatrix}e^{i(k_xx+k_yy)}. \tag{34}$$

Now imposing the continuity conditions of the wave functions at the boundaries ($x=0$ and D), lead us to the following equations:

$$1+r=\beta a+\beta b, \tag{35}$$

$$\lambda e^{i\phi}-\lambda re^{-i\phi}=\eta\lambda' ae^{i\theta}-\eta\lambda' be^{-i\theta}, \tag{36}$$

$$\beta ae^{iq_xD}+\beta be^{-iq_xD}=te^{ik_xD}, \tag{37}$$

$$\eta\lambda' ae^{i\theta+iq_xD}-\eta\lambda' be^{-i\theta-iq_xD}=\lambda te^{i\phi+ik_xD}. \tag{38}$$

Finally one can obtain the exact expression for the probability transmission as

$$T(\phi)=\frac{\cos^2\phi\cos^2\theta}{(\cos\phi\cos\theta\cos(q_xD))^2+\sin^2(q_xD)\left(\frac{1}{\eta\beta}-\lambda\lambda'\sin\phi\sin\theta\right)^2}. \tag{39}$$

This expression shows that for normal incidence, T is given by

$$T(0)=\frac{1}{1+f\sin^2(q_xD)}, \tag{40}$$

where

$$f=\frac{1-\eta\beta}{\eta\beta}. \tag{41}$$

We see that Eq. (40) is independent of the band index, λ', contrary to the expression (30) which gives the different values for transmission probability for the same values of $|V_0-E|$. Note that $T(0)$ is less than unity and, therefore, the barrier is not completely transparent, the result that we cannot see in a gapless

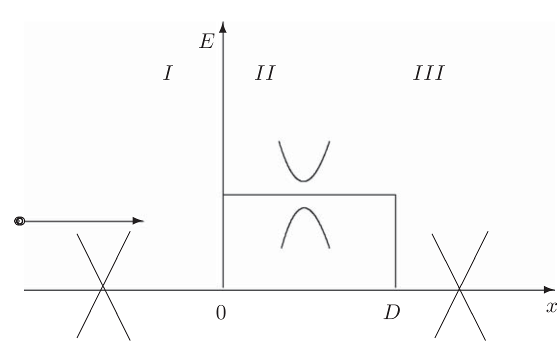

Fig. 3. A barrier of hight V_0 and width D which massless electrons, under it, acquire a finite mass.

graphene. From Eq. (39), it is obvious that for the case of $q_x = n\pi$, with n an integer, the barrier becomes completely transparent. Notice that in the limit $V_0 \to 0$ since

$$\eta\beta = \frac{q}{k}, \tag{42}$$

Eq. (40) becomes

$$T_0(0) = \frac{1}{1 + f_0 \sin^2(q_x D)}, \tag{43}$$

where

$$f_0 = \frac{k_x - q_x}{q_x} = \frac{E - \sqrt{E^2 - \Delta^2}}{\sqrt{E^2 - \Delta^2}}. \tag{44}$$

Subscribe "0" indicates that we have taken the limit $V_0 \to 0$. This result shows that transmission always remains less than unity and positive except for the case of q_x satisfying the condition $q_x = n\pi$, which results in complete transparency of the barrier.

4. Summary and discussion

In this work, by the use of two-dimensional massive Dirac equation, we first obtained the exact expression for transmission probability, T, of massive Dirac fermions in a gapped graphene across a two-dimensional potential barrier and showed that the transmission is smaller than one. We then studied tunneling of a massless electron of energy E which could acquire a finite mass of $\Delta/2v_F^2$ under an electrostatic potential barrier of hight V_0 and width D and found that the probability is independent of the band index $\lambda' = \pm 1$, contrary to the solution we obtained for probability transmission of massive Dirac fermions in gapped graphene. We also found that probability, for the barrier considered in Section 3, could not reach unity. However, it showed to be completely transparent for some values of Dq_x satisfying the relation $Dq_x = n$, with n an integer. It was revealed that, in the latter case, in the limit of $\Delta \to 0$ the transmission probability could not reach one, whereas in the limit $V_0 \to \infty$, it was approximately equal to unity. We also showed that our results do not depend on which valley Hamiltonian is used in obtaining the transmission T.

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