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Effect of a gap opening on the conductance of graphene with magnetic barrier structures

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ABSTRACT

In the present study Klein tunneling in a single-layer gapped graphene was investigated by transfer matrix method under normal magnetic field for one and two magnetic barriers. Calculations show that electron transmission through a magnetic barrier is deflected to positive angles and reduces as the magnitude of magnetic field and especially the energy gap increases. This reduction is even more significant in larger fields so that after reaching a specific value of energy gap, an effective confinement for fermions and suppression of Klein tunneling is reached particularly in normal incidence and the conductance becomes zero. Unlike one barrier, the process of tunneling through two magnetic barriers induces symmetric transmission probability versus the incident angle; even, for lower energy gaps, electron transmission probability increases which in turn reduces total conductance via proper changes in the value of the magnetic field and energy gap. In general, it is concluded that confining electrons in asymmetric transmission through one barrier is conducted better than two barriers.

1. Introduction

Graphene is a single layer of carbon atoms in a honeycomb lattice the unique electronic properties and applications in electronic devices of which has drawn much attention in recent years. The simplest approximation to express physical properties of charge carriers in graphene is the single particle model in a Tight binding approximation in which displacement dynamics of lattice atoms are neglected. This simple approximation describes many of the observed features of graphene, at least, qualitatively [1]. Considering the fact that Dirac fermions in graphene could tunnel through electrostatic barrier, one major goals is to control electron behavior using electric fields in graphene [2,3]. Experimental studies have shown that fermions of graphene could traverse long distance in micrometer scale without dispersion [4]. Therefore, confining Dirac fermions in the well and the electrostatic potential barriers created by electric fields is usually not done properly. One solution for this problem is using magnetic barriers instead of electronic potential barriers working based on wave vector filter [5]. Due to confining properties of magnetic field, various magnetic configurations and magnetic graphene superlattice have been studied regarding the control of charge carriers in graphene [6–10]. Based on some of these studies, applying strain in graphene, in low energy values, by means of pseudo vector potentials, can lead to pseudo magnetic fields so that a modest strain with triangular symmetry can create a nearly uniform magnetic field surpassing tens of Tesla which entails quantization of Landau levels [11–13]. When the magnetic field is reduced to less than critical field values, the Landau levels undergo a collapse transition and the classical behavior of Lorentz Force appears [14,15]. Notwithstanding the remarkable properties of graphene, the loss of band gap in it impedes its applicability in electronic devices based on graphene. There are various methods to create band gap in graphene one of which is forming graphene into ribbons [16–18]. It has been shown that the gap values increase by decreasing the nanoribbon width [19,20]. There are several other methods such as interaction of suitable elements and adsorption which can be used to create band gap in graphene [21–25]. Recently, it has been experimentally established that an adjustable and measurable gap can be created by using a monolayer graphene grown on SiC (0001) substrate by doping low-energy (5ev) Li^{+} ions in which the amount of gap depends on doze of Li^{+} ions [26]. Also, with Na adsorption onto bare and Ir cluster superlattice-precovered epitaxial graphene on Ir(111), a large gap adjustable up to 740 (mev) can be created [27].

Considering the fact that the effect of gap opening and its variation in graphene conductance with magnetic potential barrier has not been investigated yet, we were encouraged and inspired to investigate the effect of energy gap on the electron transmission probabil-

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ity and conductance in one and two magnetic barriers of single layer graphene.

The paper includes the following sections: Section two discusses electron tunneling through one and two magnetic barriers by transfer matrix method. The focus in section three is on total conductance and the angular dependence of transmission under a magnetic field effect. Section four represents a summary of the findings.

2. Model and method

In this section electron tunneling through a magnetic barrier is studied. The potential vector and the magnetic field for a magnetic potential barrier in the Landau gauge is as follows [10]:

$$B_z(x) = Bl_B[\delta(x+d) - \delta(x-d)]\hat{z}, \tag{1}$$

$$A_y(x) = Bl_B\Theta(d^2 - x^2)\hat{y}. \tag{2}$$

where $\Theta(x)$ is the Heaviside step function and $A_y(x)$ is the magnetic vector potential. The $l_B = \sqrt{\frac{\hbar}{eB}}$ is the typical magnetic length and D = 2d in which, D is the width of the barrier. We consider a graphene with a gap opening due to the sublattice symmetry breaking, in the presence of perpendicular magnetic field, $B_z(x)$, in such a system, the 2D massive Dirac fermions at low energy is described by the Hamiltonian

$$H = v_F\ \sigma.\left(P + \frac{e}{c}A(x)\right) + \Delta\ \sigma_z, \tag{3}$$

where P is the momentum operator, Δ is the energy gap and v_F is the Fermi velocity. Then the equation $H\Psi(x,y) = E\Psi(x,y)$ admits solutions

$$\Psi(x,y) = \begin{pmatrix}\psi_1(x,y)\\ \psi_2(x,y)\end{pmatrix}, \tag{4}$$

with $\psi_1(x,y)$ and $\psi_2(x,y)$ obeying the coupled equations,

$$v_F(\pi_x \pm i\pi_y)\psi_{2,1} = (E \pm \Delta)\psi_{1,2}, \tag{5}$$

In this equation, $\pi = P + \frac{e}{c}A$. Considering $\frac{\hbar v_F}{l_B}$ as the unit of energy, $\delta = \frac{\Delta l_B}{\hbar v_F}$, $\varepsilon = \frac{El_B}{\hbar v_F}$ and $\overline{x} = \frac{x}{l_B}$ are the units of length and $\Psi(x,y) = \phi(x)e^{ik_y y}$ in the Landau gauge, thus the following equation is obtained:

$$-i\left[\frac{\partial}{\partial\overline{x}} \pm (k_y l_B - \alpha)\right]\phi_{2,1}(x)e^{ik_y y} = (\varepsilon \pm \delta)\phi_{1,2}(x)e^{ik_y y}, \tag{6}$$

where $A_y(x) = Bl_B\Theta(d^2 - x^2)\hat{y} = Bl_B\alpha$ and

$$\alpha = \begin{cases}\alpha = 1 & |x| < d\\ \alpha = 0 & |x| > d.\end{cases} \tag{7}$$

Separating these coupled equations, the following equation is produced:

$$\left[-\partial_x^2 + (k_y l_B - \alpha)^2\right]\phi_{1,2} = (\varepsilon^2 - \delta^2)\phi_{1,2}. \tag{8}$$

In the range $-d < x < d$ electrons experience a barrier of height $[k_y + sgn(e)/l_B]^2$. The following are the wave functions in each region:

$$\phi_1 = \begin{cases}\rho_1 e^{ik_x x} + r\rho_1 e^{-ik_x x} & : \quad x < -d\\ a\rho_2 e^{iq_x x} + b\rho_2 e^{-iq_x x} & : \quad |x| < d\\ t\rho_1 e^{ik_x x} & : \quad x > d,\end{cases} \tag{9}$$

$$\phi_2 = \begin{cases}s\eta_1[e^{(ik_x x+\varphi)} - re^{-(ik_x x+\varphi)}] & : \quad x < -d\\ s'\eta_2[a\ e^{i(q_x x+\theta)} - b\ e^{-i(q_x x+\theta)}] & : \quad |x| < d\\ t\eta_1 e^{i(k_x x+\varphi)} & : \quad x > d.\end{cases} \tag{10}$$

s and s' are both +1. Solving the equation gives the eigenvalue of the dispersion relation as follows: $E = \pm\sqrt{\hbar^2 v_f^2 k_f^2 + \Delta^2}$, with energy gap Δ. We also have:

$$\rho_1 = \cos\frac{\alpha_k}{2}, \eta_1 = \sin\frac{\alpha_k}{2}\ \rho_2 = \sin\frac{\alpha_k{}'}{2}, \eta_2 = \cos\frac{\alpha_k{}'}{2}, S_i = \operatorname{sgn}(E - V(x)),$$

$$k = \sqrt{k^2{}_x + k^2{}_y}, \quad k' = \sqrt{q^2{}_x + \left(k_y - \frac{1}{l_B}\right)^2}, \tan\alpha_k = \hbar v_f\frac{(k_x^2 + k_y^2)^{1/2}}{\Delta},$$

$$\tan\alpha_k' = \hbar v_f\frac{\left[q_x^2 + \left(k_y - 1/l_B{}^2\right)\right]^{1/2}}{\Delta}, q^2{}_x + \left(k_y - \frac{1}{l_B}\right)^2 = \frac{E^2 - \Delta^2}{\hbar^2 V^2{}_f}, \tag{11}$$

$$k_x = k_f\cos\varphi, k_y = k_f\sin\varphi. \tag{12}$$

where φ is the incident angle and θ are refractive angles in barrier zone. In this study, the focus will be on Dirac point K. By applying wave functions continuity in boundaries, coefficients r, a, b and t are calculated. The transmission probability is calculated by $T = tt^*$ assuming of $\alpha = D\,k_x$ and $\beta = D\,q_x$ for one barrier using the following equation:

$$T = \frac{\cos^2\theta\ \cos^2\varphi}{\cos^2\theta\ \cos^2\varphi\ \cos^2 D\ q_x\ +\ \sin^2 Dq_x(\sin\varphi\ \sin\theta + \frac{C}{2B})}, \tag{13}$$

Where $B = \rho_1\ \rho_2\ \eta_1\ \eta_2$, $C = (\eta_1\ \rho_2)^2 + (\rho_1\ \eta_2)^2$ and:

$$\frac{C}{2B} = \frac{1}{2}\left\{\tan\frac{\alpha_k}{2}\ \tan\frac{\alpha'{}_k}{2} + co\ \tan\frac{\alpha_k}{2}\ co\ \tan\frac{\alpha'{}_k}{2}\right\}, \tag{14}$$

Conservation of energy in two regions gives the following equation:

$$\sin|\theta| = \sin|\phi| - \operatorname{sgn}(\phi)\frac{1}{k_F l_B}. \tag{15}$$

Subsequently, this ends in asymmetric transmission through one and symmetric transmission through two oppositely oriented barriers. The wave functions for two magnetic barriers are as follows:

$$\phi_1 = \begin{cases}\rho_1 e^{ik_x x} + r\rho_1 e^{-ik_x x} & : \quad x < -d\\ a\rho_2 e^{iq_{1x} x} + b\rho_2 e^{-iq_{1x} x} & : \quad x \in [-d,\ 0]\\ c\rho_2 e^{iq_{2x} x} + d\rho_2 e^{-iq_{2x} x} & : \quad x \in [0,\ d]\\ t\rho_1 e^{ik_x x} & : \quad x > d,\end{cases} \tag{16}$$

$$\phi_2 = \begin{cases}s\eta_1\left[e^{(ik_x x+\varphi)} - re^{-(ik_x x+\varphi)}\right] & : \quad x < -d\\ s'\eta_2\left[a\ e^{i(q_{1x} x+\theta_1)} - b\ e^{-i(q_{1x} x+\theta_1)}\right] & : \quad x \in [-d,0]\\ s'\eta_2\left[c\ e^{i(q_{2x} x+\theta_2)} - d\ e^{-i\left(q_{2x} x+\theta_2\right)}\right] & : \quad x \in [0,d]\\ s\eta_1 te^{i(k_x x+\varphi)} & : \quad x > d.\end{cases} \tag{17}$$

where φ is the incident angle and θ_1, θ_2 are refractive angles in environments 1 and 2 respectively. The transmission coefficient T for two barriers is calculated by applying boundary conditions. In a particular case and for the normal incident, transmission coefficient T for two barriers is calculated through:

$$T(\varphi = 0) = \frac{64(\rho_1\eta_1\rho_2\eta_2)}{A^2\ \cos^2(2q_x D) + P + Q + Z}, \tag{18}$$

In this equation: $A = 6(\rho_1\eta_1\rho_2\eta_2)^2 + (\eta_1\rho_2)^4 + (\rho_1\eta_2)^4$, $B = 2(\rho_1\eta_1\rho_2\eta_2)^2 - (\eta_1\rho_2)^4 - (\rho_1\eta_2)^4$, $C = \rho_1\eta_1^3\rho_2^3\eta_2 + \rho_1^3\eta_1\rho_2\eta_2^3$, $P = 16\ C^2\sin^2(2q_x D) + 8BC\sin(2k_x l) \times \sin(2q_x D)[\cos(2q_x D) - 1]$, $Q = B^2[1 + 2\cos(2k_x L)(\cos(2q_x D) - 1) + 1 - \cos(2q_x D)]^2$, $Z = 2AB\cos(2q_x D)\ [1 + (\cos(2q_x D) - 1)\ \cos(2k_x L)]$.

In above equations, L is the width of the well and D is the width of the barrier. Studies on magnetic barriers have revealed an asymmetric