Electronic transport for armchair graphene nanoribbons with a potential barrier*

Zhou Ben-Hu(周本胡)[a], Duan Zi-Gang(段子刚)[b],
Zhou Ben-Liang(周本良)[a], and Zhou Guang-Hui(周光辉)[a]†

[a] *Department of Physics, Hunan Normal University, Changsha* 410081, *China*
[b] *Institute of Optoelectronics, Shenzhen University, Shenzhen* 518060, *China*

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This paper studies the electronic transport property through a square potential barrier in armchair-edge graphene nanoribbon (AGNR). Using the Dirac equation with the continuity condition for wave functions at the interfaces between regions with and without a barrier, we calculate the mode-dependent transmission probability for both semiconducting and metallic AGNRs, respectively. It is shown that, by some numerical examples, the transmission probability is generally an oscillating function of the height and range of the barrier for both types of AGNRs. The main difference between the two types of systems is that the magnitude of oscillation for the semiconducting AGNR is larger than that for the metallic one. This fact implies that the electronic transport property for AGNRs depends sensitively on their widths and edge details due to the Dirac nature of fermions in the system.

Keywords: armchair-edge graphene nanoribbon, potential barrier, electronic transport

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Graphene has attracted considerable attention these years due to the successful fabrication experiment by Novoselov *et al.*[1] In graphene, the electronic energy band within the low energy regime can be described by a two-dimensional (2D) Dirac-like equation at Dirac points of the honeycomb lattice Brillouin zone.[2,3] The unique band structure of graphene with a linear dispersion relation leads to many peculiar properties such as the unconventional quantum Hall effect,[4−6] finite minimal conductivity,[7] Klein tunneling[8] and Veselago lensing.[9] Very recently, Klein tunneling through a p–n junction or a potential barrier has been widely studied[10−14] since the experimental realization[10,15] of graphene junctions. Huard *et al.*[10] have fabricated a gate-tunable barrier device from a single-layer graphene sheet, and studied the transport properties across the potential barrier. The transmission probabilities for a graphene p–n junction within steplike and smooth potentials have been calculated, respectively.[11] Katsnelson *et al.*[12] have also elucidated the dramatic difference between quantum transport of Dirac fermions in graphene and conventional 2D electrons, and have manifested that the barrier always remains perfectly transparent for particles close to the normal incidence in an infinite plane of graphene. However, the electronic transmission for graphene nanoribbons (GNRs) with potential barrier has seldom been studied. The GNRs [16−21] and dots[22] are of importance because of their electronic and transport properties heavily depending on geometry and edge details.

In this paper, we study the electronic transport property through a square potential barrier in armchair-edge GNRs (AGNRs). By using the Dirac equation[3,23] with the continuity condition for wave functions at the interfaces between regions with and without a barrier, we calculate the mode-dependent transmission probability for both semiconducting and metallic AGNRs, respectively. It is shown that, by some numerical examples, the transmission probability is an oscillating function of the height and range of barrier for both types of AGNRs, while the magnitude of the oscillations for the semiconducting case is stronger than that for metallic ones. Some new transport characteristics are obtained and compared with previous related works.[8,12]

Assuming that the edges of an AGNR are parallel to the x-axis, we begin with the Dirac equation[3,23]

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†Corresponding author. E-mail: ghzhou@hunnu.edu.cn
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$$-\mathrm{i}\,\hbar v_{\mathrm{F}}\begin{pmatrix}\sigma_x\partial_x+\sigma_y\partial_y & 0\\ 0 & \sigma_x\partial_x-\sigma_y\partial_y\end{pmatrix}\psi + V(x)\psi = E\psi \quad (1)$$

for the system, where $v_{\mathrm{F}}\approx 10^6$ m/s is the Fermi velocity and $\boldsymbol{\sigma}=(\sigma_x,\sigma_y)$ the Pauli matrices. The potential barrier $V(x,y)=V_0$ for $0< x < L$ and $0< y < W$ and $V(x,y)=0$ elsewhere, where W is the width of the GNR and L the range of the potential barrier. The four-component electronic wavefunction in Eq. (1) is $\psi=(\psi_A,\psi_B,\psi'_A,\psi'_B)^{\mathrm{T}}$, where ψ_μ (μ=A, B is the sublattice index) and ψ'_μ are the components for the two valleys, respectively. According to the translational invariance in the x-direction, the four-component wavefunction can be rewritten[23] as $\psi=\mathrm{e}^{\mathrm{i}\,k_x x}\phi(y)$ with $\phi(y)=a_n(1,z_{n,k_x},0,0)^{\mathrm{T}}+a'_n(0,0,z_{n,k_x},1)^{\mathrm{T}}+b_n(z_{n,k_x},1,0,0)^{\mathrm{T}}+b'_n(0,0,1,z_{n,k_x})^{\mathrm{T}}$, where a_n, a'_n, b_n and b'_n determined by the continuous condition at the interface are the coefficients of the n-th mode, and the complex quantity $z_{n,k_x}=\pm(k_x+\mathrm{i}\,k_n)/\sqrt{k_x^2+k_n^2}$ in which the plus sign is applied to the conduction band and the minus sign is applied to the valence band, k_x is the longitudinal wavevector and the discrete transversal wavevector $k_n=n\pi/W$ and $(n+1/3)\pi/W$ with integer n for metallic and semiconducting AGNRs, respectively. Additionally, it is worthwhile to note that in general equation (1) is also appropriate for zigzag GNRs. For zigzag GNRs the boundary conditions lead to surface waves (edge states) existing near the edge of GNRs, which complicates the analytical solution.

In order to solve the transport problem for the system, we assume that k_n is unchanged both outside and inside the potential barrier, and the mode matching at the interface does not mix the modes.[23–25] Therefore, for a unit amplitude n-th mode normally emitting from the left side, the electronic wavefunctions scattered by the potential barrier in different regions can be written as

$$\begin{aligned}\psi_{\mathrm{L}}&=(\mathrm{e}^{\mathrm{i}\,k_x x}+r_n\mathrm{e}^{-\mathrm{i}\,k_x x})\phi(y),\ \ (x<0),\\ \psi_{\mathrm{M}}&=(c_n\mathrm{e}^{\mathrm{i}\,q_x x}+d_n\mathrm{e}^{-\mathrm{i}\,q_x x})\phi(y),\ \ (0<x<L),\\ \psi_{\mathrm{R}}&=\frac{\sqrt{2}}{2}t_n\mathrm{e}^{\mathrm{i}\,k_x(x-L)}\phi(y),\ \ (x>L).\end{aligned} \quad (2)$$

In these wave functions $k_x=\sqrt{E^2/(\hbar v_{\mathrm{F}})^2-k_n^2}$ and $q_x=\sqrt{(E-V_0)^2/(\hbar v_F)^2-k_n^2}$ are the longitudinal wavevectors outside and inside the potential barrier, respectively. The real q_x corresponds to propagable modes and the imaginary q_x corresponds to evanescent modes. Moreover, the complex quantities outside and inside the barrier should satisfy the relationship of $z_{n,k_x}z_{n,-k_x}=z_{n,q_x}z_{n,-q_x}=-1$.

In Eq. (2), the coefficients of reflection r_n and transmission t_n as well as the other two c_n and d_n can be determined by continuous condition at interfaces x=0 and x=L. Unlike the Schödinger equation we only need to match the wavefunction but not its derivative. Therefore, we obtain the following four independent equations:

$$\begin{aligned}&\begin{pmatrix}1\\ z_{n,k_x}\end{pmatrix}+r_n\begin{pmatrix}1\\ z_{n,-k_x}\end{pmatrix}=c_n\begin{pmatrix}1\\ z_{n,q_x}\end{pmatrix}+d_n\begin{pmatrix}1\\ z_{n,-q_x}\end{pmatrix},\\ &t_n\begin{pmatrix}1\\ z_{n,k_x}\end{pmatrix}=c_n\begin{pmatrix}1\\ z_{n,q_x}\end{pmatrix}\mathrm{e}^{\mathrm{i}\,q_x L}+d_n\begin{pmatrix}1\\ z_{n,-q_x}\end{pmatrix}\mathrm{e}^{-\mathrm{i}\,q_x L}.\end{aligned} \quad (3)$$

Solving Eq. (3) we can obtain the transmission coefficient

$$t_n=\frac{(1+z_{n,k_x}^2)(1+z_{n,q_x}^2)}{\mathrm{e}^{\mathrm{i}\,q_x L}(z_{n,k_x}-z_{n,q_x})^2+\mathrm{e}^{-\mathrm{i}\,q_x L}(1+z_{n,k_x}z_{n,q_x})^2}, \quad (4)$$

which yields the n-th mode transmission probability $T_n=|t_n|^2$ for the system.

In what follows we present some numerical examples of the calculated transmission probability for the system according to Eqs. (3) and (4). The following parameters are used in the calculation. The width of the ribbon satisfies[3,21] the condition W=$(3N+1)a_0$ for metallic AGNR and otherwise for a semiconducting one with integer N and graphene lattice constant $a_0=2.46$ Å. The incident energy is taken[12] as $E=0.175$ eV.

In Fig. 1, we plot the mode-dependent transmission probability versus barrier height V_0 (in units of eV) for normal incidence with energy $E = 0.175$ eV and potential barrier range $L = 10$ nm. The solid curves correspond to a metallic AGNR of width $W = 28.04$ nm and the dashed curves correspond to a semiconducting AGNR of width $W = 27.92$ nm, where thick lines are for the first ($n = 1$) mode and thin lines are for the second ($n = 2$) mode, respectively. First of all, we notice that the transmission probability for AGNRs is very different from that for an infinitive graphene[8,12] which supports perfect transmission regardless of the barrier height (Klein tunneling). However, it is generally an oscillating function of the barrier height due to the quantum interference and quantum size effect of the system, but still shows some points of maximum transmission of T=1 with certain barrier height. Moreover, the bottom of each valley (minimum transmission) decreases with the increase of barrier height, and remains constant as the barrier height reaches 1.3 eV. This phenomenon can be understood via Eq. (4): the transmission probability is an oscillating function of wavevector q_x with resonant condition $q_x L = N\pi$ ($N = 0, \pm 1, \pm 2, \ldots$), but q_x is determined by V_0, so that T is also an oscillating function of V_0 with the periodicity of oscillation determined by resonance conditions. The same behaviour has been observed in Ref.[8] (see, e.g., Fig. 6 in Ref. [8]) for the double barrier and single well structures. Furthermore, from Fig. 1 we can see that the transmission probability of the system is mainly determined by the first mode because the average value of transmission for the first mode is obviously much larger than that for the second mode. Meanwhile, the transmission probability, as expected, for the metallic AGNR is larger than that for the semiconducting one with the same mode due to the zero energy gap between conduction and valence bands for the metallic AGNR. In addition, we note that the behaviour of transmission probability is analogous to that shown in Fig. 1 in the case of $V_0 < 0$ (not shown here).

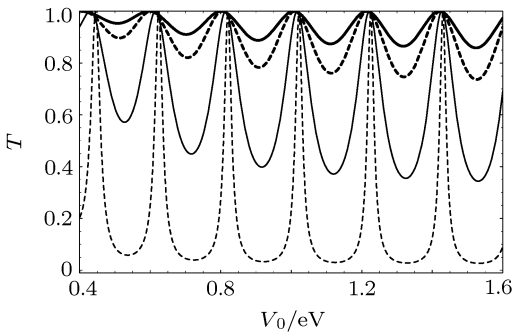


Fig. 1. Transmission probability T versus barrier height V_0 (in units of eV) for normally incident electrons with energy $E = 0.175$ eV and potential barrier range $L = 10$ nm. The solid curves correspond to a metallic AGNR of width $W = 28.04$ nm and the dashed curves correspond to a semiconducting one of width $W = 27.92$ nm, with thick lines for the first mode and thin lines for the second mode, respectively.

Figure 2 displays the transmission probability for main mode T_1 ($n = 1$) versus L (in units of nm), where the solid line is for a metallic AGNR and the dashed line is for a semiconducting one, respectively. The barrier height is taken as $V_0 = 0.285$ eV and the other parameters are the same as those for Fig. 1. As expected, T_1 is a standard oscillating function of the barrier range for both types of AGNRs. Physically, this phenomenon can be understood as: when a traveling particle satisfies the conventional resonance condition $q_x L = n\pi$, it can pass through the barrier region via resonant tunneling because of the phase accumulation. A similar result has been obtained in Ref. [26] where the incident angle is taken as 30°. Additionally, the metallic AGNR has an averagely larger transmission probability with smaller oscillating periodicity in comparison with the semiconducting one because of the different k_n for the two cases, which is consistent with the result in the previous work.[12]

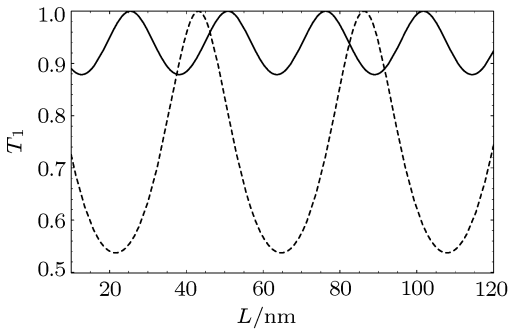


Fig. 2. Transmission probability for the main mode T_1 versus barrier range L (in units of nm) with barrier height $V_0 = 0.285$ eV, where the solid curve corresponds to a metallic AGNR while the dashed curve corresponds to a semiconducting one. Other parameters are the same as those for Fig. 1.

In Fig.3 we presents T versus V_0 (in units of eV) for a wider metallic AGNR of $W = 34.48$ nm (solid curves) and a wider semiconducting one of $W = 34.56$ nm (dashed curves), with thick lines for the first mode and thin lines for the second mode, respectively, other parameters are the same as those for Fig.1. Firstly, we can find that the transmission behaviour is analogous to Fig.1 for the narrow AGNRs.

However, the transmission probability has been much enhanced in comparison with Fig. 1. This result is as expected since the edge details become insignificant with the increase of AGNR width. If we continue to increase the width of the AGNR, the transmission probability for both types of AGNRs will tend to unity which corresponds to graphene.[8,12,26]

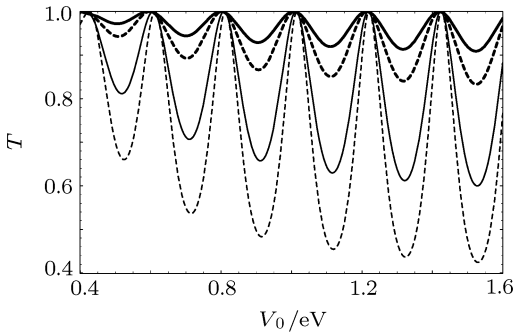


Fig. 3. Transmission probability T versus barrier height V_0 (in units of eV), where the solid curves correspond to a metallic AGNR of width W=34.48 nm and the dashed curves correspond to a semiconducting one of width W=34.56 nm, thick lines for the first mode and thin lines for the second mode, respectively. Other parameters are the same as those for Fig.1.

In conclusion, by using the Dirac equation with continuity of the wavefunctions at the interfaces, we have theoretically calculated the mode-dependent transmission probability through a square potential barrier in both metallic and semiconducting AGNRs. It has been found that the transmission probability is an oscillating function of the barrier height and range, and the magnitude of the oscillations for semiconducting AGNRs is stronger than that for metallic ones. In other words, the transmission probability of AGNRs depends sensitively on their widths and edge details, which is different from those for an infinite plane of graphene system. These size and edge effects may be helpful in the design of graphene-based nanoelectronic devices.

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