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Transmission gaps in graphene superlattices with periodic potential patterns

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ABSTRACT

The transmission probability of electrons tunneling through a graphene superlattice with periodic potential patterns is investigated using the transfer matrix method. It is found that the transmission probability as a function of incidence energy has more than one gap. The number, width and position of transmission gaps can be modulated by changing the period number, the incidence angle, the height and width of the potential. These characteristics of the transmission gaps in graphene superlattices may facilitate the development of many graphene-based electronics such as a multichannel electron wave filter.

1. Introduction

Graphene, a new allotrope of carbon, has attracted much attention both in theoretical and experimental research due to its particular electronic properties since it was experimentally fabricated by Novoselov et al. [1]. The quasiparticles in single-layer graphene are massless Dirac fermions with linear dispersion spectrum relation, which can be governed by a massless Dirac equation. Thus, graphene exhibits a multitude of novel electronic and transport properties, for instance, half-integer quantum Hall effect [2,3], finite minimal conductivity [2,4], electron–phonon interaction [5], and ultrahigh carrier mobility [6]. Another novel electronic transport property is the perfect transmission in tunneling through an arbitrarily high and wide graphene barrier at normal incidence, which is referred to as Klein tunneling [7]. Since the Klein tunneling was first studied in single barrier in graphene, the transport properties of massless Dirac fermions tunneling through the single [7–11] and double [12–15] graphene barriers have been extensively studied. When the Dirac fermions transport through a single square barrier in graphene at nonzero angle, the transmission probability as a function of incidence energy has a gap due to the appearance of evanescent waves inside the barrier [8]. The transmission gap can be controlled by the incidence angle, the height, and width of the barrier. A transmission gap also exists when the electrons transport through a trapezoidal barrier at nonzero angle [11]. These features of transmission gap in single square and trapezoidal barrier are suggested to realize an energy-dependent electron wave filter.

Recently, many studies of graphene superlattices [16–23] have been reported experimentally and theoretically. The periodic graphene superlattices can be generated by different methods, such as applying periodically gate electrodes [24] or parallel ferromagnetic metal stripes [16] on graphene to generate electrostatic potentials or magnetic barriers. The electronic transport properties and band structures of the graphene-based one-dimensional (1D) superlattices with periodic [17,18], Fibonacci [20], and Thue–Morse sequence [21] have been studied. Furthermore, the transmission gaps in graphene superlattices have also been investigated [23]. The authors studied the transmission gap in single-barrier, double-barrier and triple-barrier. It is found that the number of transmission gaps is in line with the number of barriers with different heights, and the transmission gaps can be controlled by adjusting the height and width of the barriers.

It is well known that the marked property of photonic crystals is photonic band gap, where the propagation of photons in a certain range of frequencies is strictly forbidden [25]. It is similar to the transmission gap in Dirac fermions tunneling through a graphene barrier where the transport of electrons with the incidence energy in the gap is prohibited. The photonic band gap of 1D periodic photonic crystals has been investigated with the Eigen matrix method [26], which is crucial for controlling the transport of light in photonic crystals, and can be used to design different kinds of filters [27,28]. It would be more useful for practical applications to investigate the transmission gap and control the electronic transport in gaphene superlattices with periodic potential patterns. It is notable that Berman et al. [29]

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proposed a two-dimensional (2D) graphene-based photonic crystal, which can be used as the frequency filters and waveguides for the far infrared region of electromagnetic spectrum at a wide range of the temperatures. Motivated by these studies, we investigate the transmission gaps of Dirac electrons penetrating through a graphene superlattice with periodic potential patterns at nonzero incidence angle in the present work. The dependence of transmission gaps on the period number, the height, and width of potential are discussed, respectively. These transmission gaps in graphene superlattices are potentially useful in designing an electron wave filter.

2. Theoretical model

We consider the Dirac fermions with energy E incident from the left side of the periodic potential structure at angle θ_0, with respective to the x axis, as shown in Fig. 1. The periodic structure, which can be fabricated by applying a local top gate voltage to the graphene [24], consists of elements A and B, with the period number N. The element A(B) denotes a barrier (well) with the width $d_A(d_B)$. The quasiparticles in single-layer graphene at low energy governed by the massless Dirac Hamiltonian: $\hat{H} = v_F\vec{\sigma}\cdot\vec{p} + V(x)$ in the presence of electrostatic potential $V(x)$. $\vec{p}$ is the momentum operator, $\vec{\sigma} = (\sigma_x, \sigma_y)$ is the Pauli matrices, and $v_F \approx 10^6$ m/s is the Fermi velocity. The Hamiltonian acts on a two-component pseudospinor wave function $\Psi = (\tilde{\psi}_A, \tilde{\psi}_B)^T$, where $\tilde{\psi}_A$ and $\tilde{\psi}_B$ are the smooth enveloping functions for two triangular sublattices in graphene. The wave function $\tilde{\psi}_{A,B}(x, y)$ can be expressed as $\tilde{\psi}_{A,B}(x, y) = \psi_{A,B}(x)e^{ik_y y}$ due to the translation invariance in the y direction. The wave function $\begin{pmatrix}\psi_A(x)\\ \psi_B(x)\end{pmatrix}$ at x and $x+\Delta x$

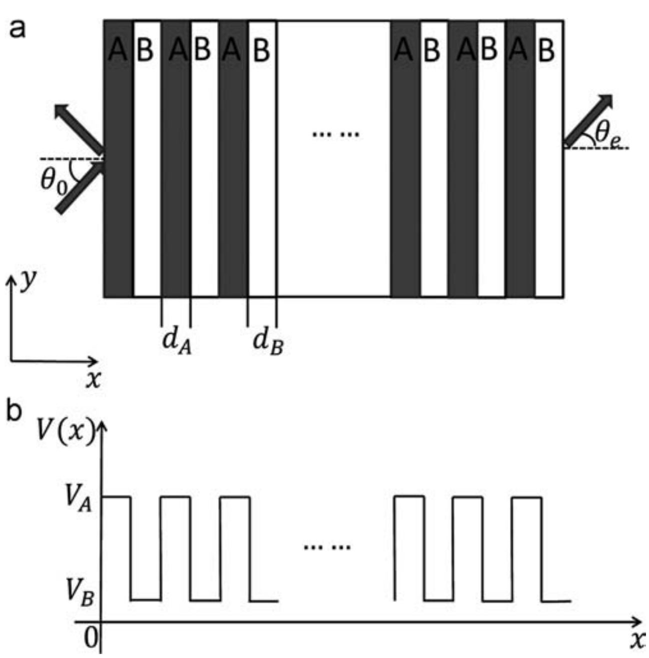

Fig. 1. (a) Schematic diagram of graphene superlattices $(AB)^N$ with one-dimensional periodic potentials, N is the period number. (b) The schematic profiles of the potential V_A and V_B.

in the jth potential can be connected with the transfer matrix [18]:

$$M_j(\Delta x, E, k_y) = \begin{pmatrix} \frac{\cos(q_j\Delta x - \theta_j)}{\cos\theta_j} & i\frac{\sin(q_j\Delta x)}{\cos\theta_j} \\ i\frac{\sin(q_j\Delta x)}{\cos\theta_j} & \frac{\cos(q_j\Delta x + \theta_j)}{\cos\theta_j} \end{pmatrix}. \quad (1)$$

Here, $q_j = \mathrm{sign}(k_j)\sqrt{k_j^2 - k_y^2}$ is the x component in the jth potential V_j for $k_j^2 > k_y^2$, or $q_j = i\sqrt{k_y^2 - k_j^2}$ for $k_j^2 < k_y^2$. $k_y = k_j \sin\theta_j$ is the y component of the wave vector $k_j = (E - V_j)/\hbar v_F$ inside the potential V_j, $\theta_j = \arcsin(k_y/k_j)$ is the angle in the jth potential. The entire transfer matrix which connects the incident and exit wave functions can be obtained

$$X = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} = \prod_{j=1}^{2N} M_j(d_j, E, k_y)$$
$$= (M_A M_B)^N = \begin{pmatrix} m_{11}u_{N-1} - u_{N-2} & m_{12}u_{N-1} \\ m_{21}u_{N-1} & m_{22}u_{N-1} - u_{N-2} \end{pmatrix}. \quad (2)$$

Here, $M_A M_B = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$, and N is the period number of this periodic potential structure. $u_N \equiv u_N(\chi) = \sin[(N+1)\zeta]/\sin\zeta$ is the Chebyshev polynomials of the second kind, and $\chi = \mathrm{Tr}[M_A M_B]/2$, $\zeta = \cos^{-1}\chi$ is the Bloch phase of the periodic system [30].

According to Bloch's theorem, the electronic dispersion at any incidence angle for infinite periodic structure is

$$\cos(K\Lambda) = \chi = \cos\zeta = \mathrm{Tr}[M_A M_B]/2$$
$$= \cos(q_A d_A)\cos(q_B d_B)$$
$$+ (\sin\theta_A \sin\theta_B - 1)\sin(q_A d_A)\sin(q_B d_B)/(\cos\theta_A \cos\theta_B) \quad . \quad (3)$$

Here, K is the Bloch wave vector, and $\Lambda = d_A + d_B$ is the length of the unit cell. When $|\cos(K\Lambda)| = |\mathrm{Tr}[M_A M_B]/2| < 1$, K is real, the Bloch wave is a propagation mode, and it corresponds to the allowed band. The forbidden gap is given by $|\cos(K\Lambda)| = |\mathrm{Tr}[M_A M_B]/2| > 1$, where K is imaginary, and the Bloch wave is a evanescent wave. Thus, $|\cos(K\Lambda)| = |\mathrm{Tr}[M_A M_B]/2| = 1$ give the boundaries of the forbidden gap, namely the transmission gap.

With the entire transfer matrix, the reflection and transmission coefficients are given by

$$r(E, k_y) = \frac{x_{22}e^{i\theta_0} - x_{11}e^{i\theta_e} - x_{12}e^{i(\theta_0+\theta_e)} + x_{21}}{(x_{22}e^{-i\theta_0} + x_{11}e^{i\theta_e}) - x_{12}e^{i(\theta_e-\theta_0)} - x_{21}}, \quad (4)$$

$$t(E, k_y) = \frac{2\cos\theta_0}{(x_{22}e^{-i\theta_0} + x_{11}e^{i\theta_e}) - x_{12}e^{i(\theta_e-\theta_0)} - x_{21}}. \quad (5)$$

Here, θ_e is the exit angle. Thus, the transmission probability of the periodic potential structure is $T = |t|^2$. In this study, we neglect the microscopic details of the interaction effects, such as the inter-valley coupling and the spin–orbit interaction. In graphene we can realize potential steps that are smooth ($d_A \gg a$), on the lattice scale $a = 1.42$ Å, therefore there is no inter-valley scattering since the distance between the valleys in reciprocal space is $|\boldsymbol{K} - \boldsymbol{K}'| \sim 1/a$ [31,32].

With the transmission probability, we can obtain the total conductance G of the system at zero temperature according to the Landauer–Büttiker formula [33]:

$$G = G_0 \int_{-\pi/2}^{\pi/2} T\cos\theta_0 d\theta_0, \quad (6)$$

where $T = |t|^2$, and $G_0 = 2e^2 E L_y/(\pi\hbar)$ is taken as the conductance unit with L_y the sample size along the y direction. The Fano factor can