Using the tight-binding approach, the electronic interlayer transport dependence on the applied biased potential in bilayer graphene was investigated. It is shown that the applied biased potential can weaken the electronic interlayer transport, with a degree determined by the energy bands of the monolayer graphene and the wavevector $k$. In addition, numerical simulation results are discussed in detail.

Graphene is one of the most active areas of research in condensed matter physics due to its unique physical and chemical properties and due to its potential applications for novel devices. Thus the electronic transport properties of monolayer graphene have been extensively studied [1–3]. Very recently, much experimental and theoretical interest has being focused on phenomena involving the electronic properties of bilayer graphene, such as hopping-resolved electron-phonon coupling [4, 5], electron screening and excitonic condensation [6], correlation effects of the Cooper pairing of electrons and holes [7], and the quantum Hall effect (QHE) in the presence of disorder [8].

It is well-known that bulk graphene has the AB (Bernal) stacking structure composed of coupled hexagonal lattices including inequivalent sublattices A and B, i.e., the nearest neighbor layers are arranged with atoms A exactly opposite to atoms B on the other layer. Many studies of bilayer graphene have been carried out on the Bernal stacking structure borrowed from that of bulk graphene [5, 9, 10]. Sophisticated techniques for the fabrication of monolayer graphene and of superlattice materials assure a possibility to fabricate a spatially separated graphene bilayer with an arbitrary separation or slippage. Indeed structures consisting of two independently gated graphene layers with common contacts and very small (0.6 nm) separation, have been fabricated and studied experimentally [11, 12]. The recent epitaxial growth technique realized twisted bilayer graphene, where two layers are stacked with a random rotation angle. Its unit cell area can be more than a thousand times as large as that of monolayer graphene, due to the slightly misoriented lattice vectors of the two layers [13]. A system of two independently contacted graphene layers separated by a 5 nm-thick SiO$_2$ barrier has been also made [14]. Thus one may imagine that isolated actual bilayer graphene systems are likely to have structures with an arbitrary separation or slippage between two monolayers and the Bernal stacking structure is a special case among them.
Bilayer graphene consists of a pair of monolayers bonded by relatively weak dimer bonds perpendicular to the plane of the monolayer sheets. In this material, both the conduction and valence bands have a low energy structure consisting of two quadratic branches separated by the energy associated with the dimer bond [15]. It is clear that a relative separation or slippage of two monolayers and doping with another element into the interlayer may influence the bands perpendicular to the plane of the monolayer sheets, such as the dimer bond, and consequently may influence the electronic interlayer transport of bilayer graphene, which is closely relate to the interlayer conductivity of bilayer graphene. Study of the electronic interlayer transport of bilayer graphene with relative slippage is of interest.

In isolated monolayer graphene, the $\sigma$ band wavefunctions do not mix with the $\pi$ band wavefunction originating from the $2p_z$ orbitals of carbon atoms, due to the fact that the $2s, 2p_x$ and $2p_y$ orbitals, which form $\sigma$ bands, are even under reflection in the plane of graphite, while the $2p_z$ orbitals are odd under reflection in the plane and have an orientation perpendicular to the plane [16]. This is why the conductance of graphene is mainly determined by the itinerating electrons of the $\pi$ bands, and the dimer bonds perpendicular to the plane of the monolayer sheets of bilayer graphene are due to the $2p_z$ orbitals.

On the theoretical level, tight-binding models are of fundamental importance, since they have been shown to capture almost all the electronic features in systems. Given the nearest neighbor hopping energy $\gamma_0$ and the onsite energy $E_p$ of the $\pi$ electrons, with the four basis Bloch sums of the $k$ wavevector built from the $p_z$ orbital of the carbon atoms A and B in the unit cell, $\Phi_{jA}(k, r_j) = (1/\sqrt{N})\sum_{m_j} e^{ikr_m} \times \phi_{jz}(r_j - d_{jA} - t_{m_j})$ and $\Phi_{jB}(k, r_j) = (1/\sqrt{N})\sum_{m_j} e^{ikr_m} \times \phi_{jz}(r_j - d_{jB} - t_{m_j})$, $j \in 1, 2$, the tight-binding model for two monolayer graphenes far away from each other (i.e., without interlayer coupling) can be described by the following Hamiltonian:

$$H = \begin{pmatrix}
E_p & \gamma_0 F(k) & 0 & 0 \\
\gamma_0 F(k)^* & E_p & 0 & 0 \\
0 & 0 & E_p & \gamma_0 F(k) \\
0 & 0 & \gamma_0 F(k)^* & E_p
\end{pmatrix},$$

(1)

where $F(k) = 1 + 2 \cos(k_x a/2) \exp(-i\sqrt{3}k_y a/2)$, and $j = 1, j = 2$ denotes the top and the bottom monolayer graphenes, respectively. In such a system the wavefunctions of the top layer do not mix with those of the bottom layer. Its eigenvalues and corresponding eigenvectors are: $E_1 = E_3 = E_p - \gamma_0|F(k)|$, $\Psi_1(k, r_1) = (1/\sqrt{2})[-(F(k)/|F(k)|)\Phi_{1A}(k, r_1) + \Phi_{1B}(k, r_1)]$, $\Psi_3(k, r_2) = (1/\sqrt{2})[-(F(k)/|F(k)|)\Phi_{2A}(k, r_2) + \Phi_{2B}(k, r_2)]$; $E_2 = E_4 = E_p + \gamma_0|F(k)|$, $\Psi_2(k, r_1) = (1/\sqrt{2})[(F(k)/|F(k)|)\Phi_{1A}(k, r_1) + \Phi_{1B}(k, r_1)]$, $\Psi_4(k, r_2) = (1/\sqrt{2})[(F(k)/|F(k)|)\Phi_{2A}(k, r_2) + \Phi_{2B}(k, r_2)]$. To study the electronic interlayer transport depending on the applied biased potential, a model of bilayer graphene with simple interlayer coupling between two monolayers, without loss of universality, is presented as follows.

It is noted that such a simplification does not substantially alter the research results.

As shown as Fig. 1, only the nearest neighbor in-plane hopping $\gamma_0$ and the nearest neighbor vertical hopping $\gamma_1$, $\gamma_2$, $\gamma_3$ are considered, which originate from the interactions
FIG. 1: (a) Schematic description of the bilayer graphene model reflecting on slippage between two monolayers. The black circle denotes atoms A, while the gray circle denotes atoms B. The top (bottom) lattice is shown by solid (dashed) lines. $\gamma_0$ is for the nearest neighbor in-plane hopping, while $\gamma_1$, $\gamma_2$, and $\gamma_3$ are respectively for the nearest neighbor vertical hoppings of an atomic orbit on the top layer with atomic orbits 1,2,3 on the bottom layer. (b) The partial top view of (a).

of the $2p_z$ orbits. In the case of atoms A in the top layer exactly opposite to atoms A in the bottom layer, i.e., there is no slippage between the two monolayers, $\gamma_2$ and $\gamma_3$ can be neglected, since they are much smaller than $\gamma_1$. While in the case of the top monolayer having a slippage relative to the bottom one, where atoms A in the top are not exactly again opposite to those in the bottom (see Fig. 1), $\gamma_2$, $\gamma_3$ must be considered together with $\gamma_1$, for they are of the same interaction order. With biased potentials applied on the bilayer graphene (the top with potential $U$ and the bottom with nil potential), the system’s Hamiltonian thus reads as

$$H = \begin{pmatrix} U + E_p & \gamma_0 F(k) & \gamma_1 & \gamma' \\ \gamma_0 F(k)^* & U + E_p & \gamma' & \gamma_1 \\ \gamma_1 & \gamma' & E_p & \gamma_0 F(k)^* \\ \gamma' & \gamma_1 & \gamma_0 F(k)^* & E_p \end{pmatrix}, \quad (2)$$

where $\gamma' = \gamma_2 \exp(-i\mathbf{k} \cdot \mathbf{t}_1) + \gamma_3 \exp(-i\mathbf{k} \cdot \mathbf{t}_2)$, $\mathbf{t}_1 = (a/2)(1, \sqrt{3})$, $\mathbf{t}_2 = (a/2)(-1, \sqrt{3})$. Based on the four eigenvectors of the Hamiltonian described in expression (1), here the Hamiltonian becomes $H = H_0 + H'$, with

$$H_0 = \begin{pmatrix} E_p + U - \eta & 0 & 0 & 0 \\ 0 & E_p + U + \eta & 0 & 0 \\ 0 & 0 & E_p - \eta & 0 \\ 0 & 0 & 0 & E_p + \eta \end{pmatrix}, \quad (3)$$
and

\[
H' = \begin{pmatrix}
0 & 0 & H'_{13} & H'_{14} \\
0 & 0 & H'_{23} & H'_{24} \\
(H'_{13})^* & (H'_{23})^* & 0 & 0 \\
(H'_{14})^* & (H'_{24})^* & 0 & 0
\end{pmatrix},
\]

where \( \eta = \gamma_0 |F(k)|, H'_{13} = \gamma_1 - \gamma'(F(k) + F(k)^*)/(2|F(k)|), H'_{14} = \gamma'(F(k) - F(k)^*)/(2|F(k)|), H'_{23} = \gamma'(F(k)^* - F(k))/(2|F(k)|), H'_{24} = \gamma_1 + \gamma'(F(k) + F(k)^*)/(2|F(k)|) \). The wavefunctions of the top layer mix with those of the bottom layer due to interlayer hoppings, \( \gamma_1, \gamma_2, \gamma_3 \).

Because of the applied biased potential and interlayer hopping, there exists electrons injecting into the bilayer graphene from and electrons outflowing to the outer electrocircuit. This means that there is electronic transport between the two sheets of graphenes.

To understand the electronic transport in monolayer graphene and bilayer graphene, the electronic properties including the transport ones of an electron with wavevector \( k \) near the Dirac cone of monolayer graphene have been widely explored [17–19]. The conductivity of a material is due to the electrons in the conduction bands and holes in the valence bands. They play different roles in the conductivity, related to their wavevector \( k \). As a result of thermal electrons excited into conduction bands, a valence band is not completely filled again, being left with a small quantity of holes in it. Accordingly, investigation of the transport in the material of electrons with different wavevectors \( k \) and in different energy bands is nontrivial.

From now on we explore the electronic interlayer transport in the bilayer graphene biased with an applied potential, paying attention to the evolution of a state vector which is initially localized on a layer (for example on the bottom layer). Diagonalizing the Hamiltonian \( H \) described by expressions (3) and (4), the system’s exact eigenvalues \( \varepsilon_l \) and eigenvector \( |\xi_l(k)\rangle \) can be obtained, thereby the exact evolving state \( |\psi(k, t)\rangle \), originating from an arbitrary initial state, \( |\psi(k, 0)\rangle = a|\Psi_3(k)\rangle + b|\Psi_4(k)\rangle \), where \( a^2 + b^2 = 1 \), is obtained as \( |\psi(k, t)\rangle = \sum_l (\xi_l|\psi(k, 0)\rangle \exp(-i\varepsilon_l t/\hbar)|\xi_l\rangle \). Consequently the probability \( P_{top}(t) \), with which at time \( t \) the electron initially localized on the bottom layer is found on the top layer, is

\[
P_{top}(t) = (\sum_l (\xi_l|\psi(k, 0)\rangle \exp(-i\varepsilon_l t/\hbar)|\Psi_2(k)|\xi_l\rangle)^2 + (\sum_l (\xi_l|\psi(k, 0)\rangle \exp(-i\varepsilon_l t/\hbar)|\Psi_2(k)|\xi_l\rangle)^2) \text{ and thus the averaged probability over time } t \text{ is}
\]

\[
\langle P_{top} \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T P_{top}(t) dt = \sum_l (\langle \xi_l|\psi(k, 0)\rangle \langle \Psi_1(k)|\xi_l\rangle)^2 + \sum_l (\langle \xi_l|\psi(k, 0)\rangle \langle \Psi_2(k)|\xi_l\rangle)^2. \tag{5}
\]

To get the evolving \( |\psi(k, t)\rangle \), instead of diagonalizing the Hamiltonian \( H \), we here, using the fourth order Runge-kutta method, numerically integrate the Schrödinger equation, \( i\hbar \frac{d|\psi(k, t)\rangle}{dt} = H|\psi(k, t)\rangle \), where \( H \) is depicted by expressions (3) and (4), and with the initial state \( |\psi(k, 0)\rangle = |\Psi_3(k)\rangle \) or \( |\psi(k, 0)\rangle = |\Psi_4(k)\rangle \). In the course of simulation, the electron’s charge \( e \) denotes the energy scale wherewith to scale time as \( \hbar/e \). The onsite energy is set to \( E_F = -1.0 \), and for convenience the hopping energies \( \gamma_0 = -0.1, \gamma_1 = \gamma_2 = \gamma_3 = -0.01 \). This reflects the fact that vertical hopping is much smaller than in-plane hopping.
FIG. 2: Electronic interlayer transport in the bilayer graphene in the absence of an applied biased potential. The transport probabilities $P_{\text{top}}$ from the bottom layer to the top layer of an electron initially on the bottom layer, with initial state $|\psi(k,0)\rangle = |\Psi_4(k)\rangle$, are functions of time $t$ corresponding to the wavevectors $k = (0,0), (\pi/3a,0), (\pi/a,0), (4\pi/3a,0)$, respectively. The circles, the stars, the squares, and the triangles respectively are for $k_x = 4\pi/3a, \pi/a, \pi/3a$, and 0.

in multilayer graphene. Other cases will be discussed at the end of this paper. We found that taking the time step $\Delta t = 0.01$ and integrating this system’s Schrödinger equation till $t = T = 10^5$ (i.e., $0 \leq t \leq T = 10^7\Delta t$) is adequate to compute the averaged probability $\langle P_{\text{top}} \rangle$ in Equation (5), which characterizes the electronic transport from the bottom layer to the top layer.

The bilayer graphene without an applied biased potential is considered first. In this case (i.e., $U = 0$), Fig. 2 shows that an electron located initially at the bottom layer having an initial state $|\psi(k,0)\rangle = |\Psi_4(k)\rangle$ will transport into the top layer, and the transport probability $P_{\text{top}}$ is a sine-like function of time $t$ with a cycle determined by the wavevector $k$. The more longer is the cycle, the more slowly does the electron propagate between the two layers. Fig. 2 also shows that at the special K-point ($k = (4\pi/3a,0)$, named as the Dirac point) of the Brillouin zones, $P_{\text{top}}$ is very tiny and has a very long cycle (but less than $1.0 \times 10^5$, found by computation). This means that electrons at the K-point in Brillouin zones almost do not participate in interlayer transport. This can be theoretically analyzed. At the Dirac point the four eigenvalues of $H_0$ are quadruply degenerate, with $E_1 = E_2 = E_3 = E_4 = E_P$ and the four eigenstates are $\Psi_1(k, r_1) = \Phi_{1A}(k, r_1)$, $\Psi_2(k, r_1) = \Phi_{1B}(k, r_1)$, $\Psi_3(k, r_2) = \Phi_{2A}(k, r_2)$, $\Psi_4(k, r_2) = \Phi_{2B}(k, r_2)$. Furthermore, the Hamiltonian $H$ in expression (4) which mixes these four wavefunctions is weakest, so that the energy contribution to the energy levels $\varepsilon_l$ of the Hamiltonian $H$ as well as the mixing of $\Psi_l$, $\{l = 1, 2, 3, 4\}$ in the eigenstates $|\xi_l\rangle$ of $H$ are least ($\langle \xi_l | \psi(k, 0) \rangle \approx 0$ and 1; 0 for $l = 1, 2, 3, 1$ for $l = 4$) for this case. Based on the evolving state $|\psi(k,t)\rangle = \sum_l \langle \xi_l | \psi(k,0) \rangle \exp(-i\varepsilon_l t/h)|\xi_l\rangle$, one thus can see why an electron at or near the K-point in the Brillouin zones almost does not participate in interlayer transport and the transport probability function of time $t$ has
With a biased potential $U$ applied on two layers, we get the functions of the transport probability $P_{\text{top}}$ for an electron with an initial state $|\psi(k,0)\rangle = |\Psi_4(k)\rangle$ propagating from the bottom layer to the top layer. Fig. 3 shows that the magnitudes of $P_{\text{top}}$ are of the order of $10^{-3}$ in the cases of $k = (0, 0), (\pi/3a, 0), (\pi/a, 0)$, and $(4\pi/3a, 0)$, thereby illuminating that an applied biased potential shall weaken the interlayer transport. Also, Fig. 3 reveals that the cycles of transport probability for different $k$ are almost equal to each other. This can be understood according to first-order perturbation theory, as that under the same perturbation the more the difference between the energy levels of $H_0$, the less energy the levels obtain contributed by the perturbation $H'$. Therefore, the energy levels $|\varepsilon_l\rangle$ are mainly determined by $E_P$ and $U$, and the annexations to the energy levels by perturbations which are related to $k$ are weakened by $U$, with which $P_{\text{top}}$ almost having the same cycle can be explained. Similarly, as the analysis for the transport probability cycle, $U$ weakens the effect of $H'$ on $H$ and thus decreases the mixing of $\Psi_l, \{l = 1, 2, 3, 4\}$ in the eigenstates $|\xi_l\rangle$ of $H$. That is why in the presence of $U = -1.0$, the transport probability is smaller than that in the case of $U = 0$.

The above considerations are for some $k$ in the line along the $x$-direction in the Brillouin zone. For adequately describing the transport probability depending on $k$ and on the applied biased potential $U$, the averaged probability $\langle P_{\text{top}} \rangle$ as functions with respect to $\theta$, with which $k = \pi/2a(\cos \theta, \sin \theta)$, are computed respectively corresponding to different $U$ with initial state $|\psi(k,0)\rangle = |\Psi_3(k)\rangle$ or initial state $|\psi(k,0)\rangle = |\Psi_4(k)\rangle$. Fig. 4a shows that in the absence of an applied biased potential ($U = 0$), an electron initially localized at the bottom layer with an initial state $|\psi(k,0)\rangle = |\Psi_3(k)\rangle$ will transport to the top layer...
at an averaged probability $\langle P_{\text{top}} \rangle$ being equal to about 0.5. $\langle P_{\text{top}} \rangle$ slightly changes with $\theta$. This means that at the identical condition all $k$ with $|k| = \pi/2a$ in the Brillouin zone will transport to the top layer almost at the same averaged probability. In the case of $U = -0.5$, that is, the bilayer graphene was applied with a positive biased voltage, an electron at the bottom with a state $|\psi(k,0)\rangle = |\Psi_3(k)\rangle$ almost does not transport to the top layer in the case of $|k| = \pi/2a$. While for negative biased voltage, i.e., $U = 0.5$, the averaged probability $\langle P_{\text{top}} \rangle$ of an electron with its wavevector $|k| = \pi/2a$ is a function of $\theta$, which markedly changes with $\theta$. Fig. 4b is for an electron initially localized at the bottom layer with an initial state $|\psi(k,0)\rangle = |\Psi_4(k)\rangle$ under the same conditions to that depicted as Fig. 4a. In contrast to Fig. 4a, with $|\psi(k,0)\rangle = |\Psi_4(k)\rangle$, $\langle P_{\text{top}} \rangle$ are much less when the bilayer graphene was negatively applied with a biased voltage ($U = 0.5$) than that when positively applied with a biased voltage ($U = -0.5$), and $\langle P_{\text{top}} \rangle$ markedly changes with $\theta$ when $U = -0.5$. To analyze theoretically the above phenomena, we denote the four energy levels of $H_0$ in expression (3) as $E_j^{(0)}$, $j = 1, 2, 3, 4$, whereby $E_1^{(0)} = E_P + U - \eta$, $E_2^{(0)} = E_P + U + \eta$, $E_3^{(0)} = E_P - \eta$, and $E_4^{(0)} = E_P + \eta$. Applying a positive biased voltage to the system ($U < 0$) just increases the energy difference between the two levels $E_1^{(0)} - E_3^{(0)} = U$ and $E_2^{(0)} - E_4^{(0)} = U + 2\eta$, in term of the first-order perturbation theory, wherefore decreases the commixture of $|\Psi_3(k)\rangle$, $|\Psi_1(k)\rangle$ and $|\Psi_2(k)\rangle$. While for the energy difference of two levels $E_1^{(0)} - E_4^{(0)} = U - 2\eta$ and $E_2^{(0)} - E_3^{(0)} = U$, the decrease of the commixture of $|\Psi_4(k)\rangle$, $|\Psi_1(k)\rangle$ and $|\Psi_2(k)\rangle$ by $U < 0$ is less than that of the former.
Using the evolving state $|\psi(k,t)\rangle = \sum_l \langle \xi_l | \psi(k,0) \rangle \exp(-i\varepsilon_l t/\hbar) |\xi_l\rangle$, one can conclude that in the case of $U < 0$ the averaged probability $\langle P_{\text{top}} \rangle$ of an electron from the bottom layer to the top layer is smaller when it has an initial state $|\psi(k,0)\rangle = |\Psi_3(k)\rangle$ than when it has an initial state $|\psi(k,0)\rangle = |\Psi_4(k)\rangle$. In addition the degree of change of $\langle P_{\text{top}} \rangle$ with $\theta$ can be understood based on this analysis. Clearly, there is no requirement to repeat such an analysis on the case of $U > 0$. As shown in Fig. 5, with the continued increase of the biased voltage, there will no electron transport into the top layer, implying that the interlayer electronic conduction of bilayer graphene coming from the interlayer hoppings $\gamma_1, \gamma_2, \gamma_3$ will be nought.

Up to now, we have considered the electronic interlayer transport for electrons with some wavevectors $k$, such as $k$ in the line along the $x$-direction and for all $k$ meeting $|k| = \pi/2a$. It is noted that a similar results will be shown for electrons with other wavevectors $k$ in the Brillouin zone. In addition, the model studied here for bilayer graphene is that the top layer only moved symmetrically with a very small slippage relative to the bottom layer, consequentially the interlayer hopping energies were set to $\gamma_1 = \gamma_2 = \gamma_3$, especially $\gamma_2 = \gamma_3$. This is why the functions of averaged probability $\langle P_{\text{top}} \rangle$ with respect to the angle $\theta$ in Fig. 4 and Fig. 5 displays some symmetry in the Brillouin zone. We here point out that for other models with different hopping energies, similar results also hold, excepting that the $\langle P_{\text{top}} \rangle$ does not show the symmetry any more in the Brillouin zone when the top layer only moved unsymmetrically relative to the bottom layer. As discovered in the paper [4, 5], the interlayer hopping can induce the splitting of the Dirac point. We found in our model the splitting $\Delta E \approx 4\gamma_1\gamma_2/U$ in the cases $U \gg \gamma_1$ and $U \gg \gamma_2$, therewith the Hamiltonian $H' \equiv \{H_0\}$ acts as a perturbation of the Hamiltonian $H_0$. This means that the applied voltage not only influences the electronic interlayer transport but also works on the electronic intralayer transport in bilayer graphene, and the splitting of the Dirac point decreases with an increase
of the applied voltage. Accordingly, we conclude that increasing the biased voltage between the two layers can improve the intralayer electronic conductivity of bilayer graphene.

In summary, we have studied the electronic interlayer transport of bilayer graphene influenced by biased voltage between its two layers. It has been found that the applied biased potential can weaken the electronic interlayer transport, and with the continuous increase of the applied biased potential, the changes of interlayer transport probability with the wavevectors $k$ become less and less, finally the electronic interlayer transport coming from the interlayer hopping energies will be nought. These results with their associated detailed discussions are useful for understanding the electronic conductivity of bilayer graphene and bring forward a way to control the electronic conductivity of bilayer graphene: increasing the biased voltage between two layers of bilayer graphene can decrease the interlayer electronic conductivity contributed by the interlayer hopping energies, but at same time improves its intralayer electronic conductivity.

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