Control over band structure and tunneling in bilayer graphene induced by velocity engineering

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Abstract
The band structure and transport properties of massive Dirac fermions in bilayer graphene with velocity modulation in space are investigated in the presence of a previously created band gap. It is pointed out that velocity engineering may be considered as a factor to control the band gap of symmetry-broken bilayer graphene. The band gap is direct and independent of velocity value if the velocity modulated in two layers is set up equally. Otherwise, in the case of interlayer asymmetric velocity, not only is the band gap indirect, but also the electron–hole symmetry fails. This band gap is controllable by the ratio of the velocity modulated in the upper layer to the velocity modulated in the lower layer. In more detail, the shift of momentum from the conduction band edge to the valence band edge can be engineered by the gate bias and velocity ratio. A transfer matrix method is also elaborated to calculate the four-band coherent conductance through a velocity barrier possibly subjected to a gate bias. Electronic transport depends on the ratio of velocity modulated inside the barrier to that for surrounding regions. As a result, a quantum version of total internal reflection is observed for thick enough velocity barriers. Moreover, a transport gap originating from the applied gate bias is engineered by modulating the velocities of the carriers in the upper and lower layers.

1. Introduction
Charge carriers in monolayer graphene at low energies, near the neutrality point, are described by Dirac fermions with a velocity that is independent of wavelength [1]. This unique property proposes an analogy between Dirac fermions and electromagnetic or mechanical waves in optics and acoustics. Furthermore, this brings several unusual electronic properties such as anomalous integer [2] and fractional [3] quantum Hall effects, electronic focusing by means of a rectangular potential barrier (Veselago lensing) [4], Klein tunneling [5, 6] and minimal conductivity [7]. Spatial modulation of wave velocity has been studied in optics, acoustics and recently in photonic crystals [8]. The idea can also be applied for Dirac fermion waves by defining a velocity barrier as the region in which the Fermi velocity differs from that in the surrounding background. In analogy with optics, some optical rules are expected to be valid for massless Dirac fermion waves propagating in monolayer graphene sheets [9].

There are several ways to engineer the Fermi velocity ($v_F$) by means of a control over the electron–electron interaction in graphene. Enhancement in the electron–electron interaction induces an increase in the Fermi velocity [10]. Furthermore, an enhancement in $v_F$ which is logarithmic in the carrier concentration $n$ has been established in experiments and also described by the renormalization group theory [11]. Modifications of curvature of graphene sheet [12], periodic potentials [13] and dielectric screening [14, 15] are some of the propositions for engineering $v_F$ via the electron–electron interaction. The $v_F$ of graphene is inversely proportional to the dielectric constant of the environment embedding the graphene sheet [16]. Structures with velocity modulation in space can be also made by application of appropriate doping [17] or placing a grounded metal plane as a screening plane close to the graphene [18]. In the presence of the
screening planes, the speed of carriers is smaller than the speed at an isolated graphene sheet. Recently, in a 2D electron gas, an artificial graphene has been proposed by modulating a periodic potential of honeycomb symmetry [19]. Electrons in artificial graphene sheets behave like massless Dirac fermions with a tunable Fermi velocity.

The electronic properties of monolayer graphene sheets with spatial modulation of the Fermi velocity have been investigated in the literature [9, 18, 20–22]. However, the electronic properties in bilayer graphene (BLG) with an interlayer asymmetric velocity have not been elucidated in detail so far. There are numbers of different experiments in which a controllable direct band gap is observed in gated bilayer graphene [23–26]. However, the amount of current in the off-state still remains high [25, 27–29]. This off-current has been attributed to several sources [27] such as edge states [30], the presence of disorder [31], and coexistence of massive and massless Dirac fermions in twisted AA-stacking bilayer graphene grown on SiC [29, 32]. Strain is the other known factor which controls the band gap in BLG [33, 34].

In this work, we point out that the velocity modification in symmetry-broken BLG, as an inevitable experimental factor, is able to control the band gap. In the absence of the gate bias $\delta = 0$, symmetric or asymmetric velocity modulation in two layers is not able to create a gap in the band structure. However, the previously created gap $\delta \neq 0$ can be controlled by the ratio of modulated velocity in the upper layer to the lower layer $\eta$. The band gap is direct if the velocity of itinerant quasi-particles in each layer is set up equally. This gap is independent of velocity, while the momentum attributed to the band gap is inversely proportional to the velocity. On the other hand, the band gap is indirect for non-equal velocities modulated in layers. In this case, the band structure and subsequently the band gap are controlled by $\eta$. The shift of momentum from the conduction band edge to the valence band edge depends on the gate bias and velocity ratio. Moreover, the electron–hole symmetry fails when $\eta \neq 1$.

This kind of control over the band structure, which is induced by different velocity modulations in each layer, opens up the possibility of new device applications in nanoelectronics. More importantly, in a BLG under application of gate bias, experiments have to consider the transition of direct to indirect band gap. This transition can be induced by modification of velocity in layers originating from several experimental requirements such as coating a metallic gate electrode, changing carrier concentration by application of a gate voltage, strain etc.

To manifest such a control over the gap, we develop a transfer matrix approach to investigate transport properties through the velocity barrier subjected to a gate bias in BLG. A schematic diagram of the proposed system is presented in figure 1, which indicates simultaneous velocity and electrostatic junction. The proposed method is based on a four-band Hamiltonian for AB stacking [35, 36]. As a result, similar to monolayer graphene [9, 18, 20–22], a total internal reflection occurs for Dirac fermion waves hitting a thick barrier at angles of incidence greater than a critical angle. Moreover, it is observed that the transport gap depends on the velocity ratio $\eta$ at large gate bias. This gap is induced by application of a symmetry breaking factor in the barrier region.

We organize this paper as follows. In section 2, we present the four-band Hamiltonian and a general formula for deriving the spectrum in the presence of velocity modulation in addition to vertically applied gate bias. Then in section 3 we switch to calculate transport properties through a velocity junction possibly subjected to an external gate bias in generic form. Finally, the last section includes the results.

2. Hamiltonian and band structure in presence of interlayer asymmetry

The four-band Hamiltonian of bilayer graphene close to the Dirac point (i.e. the valley of the K point, say) for AB stacking is described as follows:

$$H = \begin{pmatrix} -i\hbar v_0 (\sigma \cdot \nabla)^\dagger + V_0 I & F \\ F & -i\hbar v_d (\sigma \cdot \nabla) + V_d I \end{pmatrix}$$

where

$$F = \begin{pmatrix} t & 0 \\ 0 & 0 \end{pmatrix}, \quad -i\hbar v \sigma \cdot \nabla = \begin{pmatrix} \pi^\dagger \\ \pi \end{pmatrix}$$

and $I$ is the unit matrix. Here, $\pi = -i\hbar(\partial_x - k_x)$, $t = 390$ meV is the coupling energy between the layers, $V_0 = V_0 + \delta$ and $V_d = V_0 - \delta$ describe an asymmetric factor which can be applied by a vertical gate bias or doping. This interlayer asymmetry emerges as a difference between on-site energies belonging to each layer. Another interlayer asymmetry can be induced by different modulations in the velocity of itinerant quasi-particles in the upper and lower layers, $v_u = \xi_d v_F$ and $v_d = \xi_d v_F$ respectively, $v_F$ is the commonly Fermi velocity used for graphene. $V_0$ is the gate voltage applied on both
layers setting up to zero. $2\delta$ is the potential difference between the upper and lower layers induced by a gate bias or doping. The eigenfunction of the above Hamiltonian [35] is written as $\Psi = (\psi_B^u, \psi_B^d, \psi_A^u, \psi_A^d)^\top$. By solving the eigenvalue equation of $H\Psi = E\Psi$, the band structure can be calculated in the gapless case or in the presence of previously applied gate bias.

At the same time as vertical gate bias is present, velocity may be experimentally modulated in each layer of BLG. In a gapped BLG, we will show that there is a possibility for engineering the previously created gap by using a velocity modulation in each layer. In the presence of a gate bias accompanied by an interlayer asymmetry in velocity, the BLG’s spectrum can be extracted from the following equation, which presents $k(E)$.

$$k(E^2) = [a \pm \sqrt{a^2 - b}] / v_u$$

where $a(E, \eta, \delta) = \eta^2(E - \delta)^2 + (E + \delta)^2$ and $b(E, \eta, \delta) = (E^2 - \delta^2)(E^2 - \delta^2 - t^2)$.

If the gate voltage is nonzero $V_0 \neq 0$, functions of $a$ and $b$ in the above equation depend on $\varepsilon = E - V_0$ instead of $E$. Based on the velocity ratio ($\eta$) and in the presence of a gate bias ($2\delta$), we will indicate that BLG has two different behaviors. For $\eta = 1$ BLG behaves as a semiconductor with direct band gap, while for $\eta \neq 1$ it behaves as a semiconductor with indirect band gap. In the case of $\delta = 0$, independent of $\eta$, there is no gap in BLG. Bulk band structure calculated by the above equation is shown for $\delta = 0$ in figure 2 and for $\delta \neq 0$ in figures 3 and 4(a).

To investigate the behavior of the energy gap $E_{\text{gap}}$, one can simply derive the following conditions to give the extremum points of $E(k)$. Based on equation (2), there are two possibilities for the energy gap $E_{\text{gap}}$.

$$E = \pm \sqrt{\varphi(k) + (-1)^\varepsilon \sqrt{\varphi^2(k) - v_{u, d}^2 k^4}}$$

where $\varepsilon = 1$ and $2$ are attributed to the low and high energy bands, respectively. In the case of $\varepsilon = 1$, there is no band gap at the Fermi Dirac point ($k = 0$). The whole spectrum is robust against the exchange of $v_u$ to $v_d$. This robustness can also be observed for $\varepsilon = 2$.
The chiral symmetry is conserved even though quasi-particles have different velocities in each layer. In this case, modulation of velocities in each layer just changes the effective mass of the quasi-particles. Figure 2 shows the energy bands of BLG with different velocities in each layer. The band structure is symmetric and behaves as a parabolic form. As a conclusion, without any application of potential difference, only interlayer asymmetry in velocity is not able to break the electron–hole symmetry.

2.2. Band structure in presence of interlayer asymmetry in potential but symmetry in velocity: direct band gap

In the presence of an interlayer asymmetric factor such as an external gate bias ($\delta \neq 0$) and in the special case of the same velocities set up on each layer ($v_u = v_d = v$ ($\eta = 1$)), the four-band spectrum is described as [27]

$$E^2 = (vk)^2 + \xi^2 + t^2/2 + (-1)^{\delta} \times \sqrt{2}\|vk\|^2 (4\eta^2 + t^2) + t^4/4 + k^2. \quad (5)$$

As shown in figure 3, the low energy band $\epsilon = 1$ displays a 'Mexican hat' shape. Despite turning the external gate bias on, the band structure still remains symmetric, giving rise to electron–hole symmetry. The functions of $a(E, \delta)$, $b(E, \delta)$ defined in equation (2) are independent of $\eta$. Therefore, the band gap is independent of the velocity which is modulated in layers. The requisite condition for deriving the band gap ($b = a^2$ in equation (3)) results in a symmetric solution for the conduction and valence band edges,

$$E_c = -E_v = \frac{\delta}{\sqrt{4\delta^2 + t^2}} \quad \forall k \neq 0. \quad (6)$$

Therefore, the band gap is written as $E_{gap} = 2E_c$. At $k = 0$, the gap is fixed to the value $2\delta$. Because $a(E_c) = a(E_v)$, one can conclude that the momenta of the conduction and valence band edges emerge at the same point $k_c = k_v = k_{gap}$ from the center of the valley.

$$k_{gap} = \pm \frac{2\delta}{\sqrt{4\delta^2 + t^2}} \frac{1}{\sqrt{\xi^2 + 4\delta^2}}. \quad (7)$$

Consequently, the band gap is direct and the momentum attributed to the gap is inversely proportional to the velocity $\xi$. For the limit of low external gate bias $\delta \ll t$, the band gap tends to the gate bias $E_{gap} \rightarrow 2\delta$. However, for large potential differences $\delta \gg t$, the band gap tends to saturate at the interlayer hopping energy $E_{gap} \rightarrow t$. For both limits, the momentum attributed to the band gap behaves as $k_{gap} \propto 2\delta/\nu$. For the case of slower velocity $\xi < 1$, the effective mass at the conduction and valence band edges is heavier than the effective mass for faster velocity $\xi > 1$.

2.3. Band structure in presence of interlayer asymmetry in potential and velocity: indirect band gap

In this case, interlayer asymmetry is applied on both the electrostatic potential and also the velocity of itinerant quasi-particles ($v_u \neq v_d$). In the case of $\eta \neq 1$ and $\delta \neq 0$, there
is an asymmetry between the conduction and valence bands of the spectrum, giving rise to electron–hole asymmetry [37]. Consequently, the conduction and valence band edges appear at asymmetric energy points measured from the band center \( E = 0 \). As a result, the momentum attributed to the conduction and valence band edges emerges at different points, \( k_c \neq k_v \). Therefore, the band gap is indirect. The shift of momentum from the conduction band edge to the valence band edge \( \Delta k = k_v - k_c \) depends on the velocity in each layer. Although the band gap just depends on the velocity ratio \( \eta \), in a fixed velocity ratio the whole feature of the spectrum is sensitive to both values of velocity attributed to the upper and lower layers. Let us set the velocity of the lower layer to be fixed as \( \xi_u = 1 \) while \( \xi_u \) is tunable. The lower and upper layers are characterized by the electrostatic potential of \( -\delta \) and \( \delta \), respectively.

The asymmetric band structure is represented in figure 4(a) for three values of velocity of the upper layer \( \xi_u \). Although the band structure is asymmetric, its form preserves the ‘Mexican hat’ shape. In appendix A, we have provided a comparison between the electron–hole asymmetry arising from the full Hamiltonian of BLG and the dominant Hamiltonian which is considered in this work.

Figure 4(b) shows the momentum attributed to the conduction \( k_c \) and valence \( k_v \) band edges and also their momentum shift \( \Delta k \) in terms of \( \xi_u \). As clearly observed, both \( k_c \) and \( k_v \) decrease with \( \xi_u \). Moreover, their curves intersect each other at \( \eta = 1 \), which results in the direct band gap. However, for all values of \( \eta \neq 1 \), the band gap is indirect. For \( \xi_u < 1 \), the momentum shift of \( k_c \) away from the Dirac point is larger than the momentum shift of \( k_v \).

By finding roots of equation (3), the conduction and valence band edges are computed in terms of system parameters. Figure 4(c) indicates the dependence of \( E_c, E_v \) and also \( E_{\text{gap}} \) on the velocity ratio \( \eta \). The curves related to \( E_c \) and \( E_v \) never intersect each other. In all ranges of \( \eta \), \( E_c > E_v \). So BLG always behaves as a semiconductor, not a metal or semi-metal. The energy gap has a maximum at \( \eta = 1 \) in which the gap is direct. A sharp variation of \( E_{\text{gap}} \) with \( \eta \) is seen for the range of \( \eta < 1 \). Parameters \( \eta_1^{cr} \) and \( \eta_2^{cr} \) are those critical velocity ratios at which \( E_c \) or \( E_v \) crosses the band center \( E = 0 \). The curvature width of function \( E_{\text{gap}}(\eta) \) is measured by \( \Delta n^{cr} = \eta_1^{cr} - \eta_2^{cr} \). The critical velocity ratio for the valence and conduction band edges is derived in the following form: \( \eta_1^{cr} = 1 + 2(t/\delta)^2(1 + \sqrt{1 + (\delta/t)^2}) \). In both limits of \( \delta \ll t \) and \( \delta \gg t \), the width of the peak which emerges in \( E_{\text{gap}}(\eta) \) tends to \( \Delta n^{cr} \rightarrow 2t/\delta \). As a conclusion, for large gate bias \( \delta \), there is a sharp variation in the energy gap as a function of the velocity ratio. For large velocity ratio \( \eta \rightarrow \infty \), the asymptotic solution of equation (3) for the conduction band edge is \( E_c \rightarrow \delta \). In this limit, the momentum attributed to the conduction band edge behaves as a power law with \( v_0 \); \( k_c \rightarrow 2\delta/v_0 \). In the opposite limit of \( \eta \rightarrow 0 \), the asymptotic solution for the valence band edge is \( E_v \rightarrow -\delta \). So, the momentum attributed to the valence band edge tends to a constant, \( k_v \rightarrow 2\delta/v_0 \).

Although the energy gap increases with the external gate bias, as shown in figure 5(a), the energy gap is controllable by means of the velocity ratio at large \( \delta \). In fact, for \( \delta \gg t \), the band gap saturates with the gate voltage at a value which is proportional to the interlayer coupling \( (t) \). In this limit, by applying the approximation of \( (|E^2 - \delta^2| \gg F) \) in equation (3), one can analytically derive that the saturated band gap at \( \delta \gg t \) behaves with the velocity ratio as follows:

\[
E_{\text{gap}}^{sat}(\eta) = \frac{2\sqrt{\eta}}{\eta + 1} t. \tag{8}
\]

In the special case of \( \eta = 1 \), the band gap saturates at \( E_{\text{gap}}(\eta = 1) \rightarrow t \). As shown in the inset of figure 5(a), numerical calculations completely confirm this analytical derivation. The momentum shift \( \Delta k \), which measures to what extent the gap is indirect, can be manipulated by using the gate bias. Figure 5(b) represents the momentum shift from \( k_c \) to \( k_v \) in respect of the gate bias for several values of \( \xi_u \). This momentum shift from \( k_c \) to \( k_v \) increases with the gate bias. If we transform the velocity ratio as \( \eta \rightarrow 1/\eta \), in the spectrum feature, the conduction band will be exchanged with the valence band. Furthermore, based on equation (3), the band gap is robust against transformation of \( \eta \rightarrow 1/\eta \).

In addition to the direct measurements of the spectrum, the dependence of the energy gap on the velocity ratio can be manifested in transport properties through a velocity junction.
3. Transport properties across non-uniform potential and velocity junctions

Let us consider a BLG sheet in which the velocity of itinerant quasi-particles in the upper and lower layers varies in space; represented as \( v_\alpha(\vec{r}) \) and \( v_\delta(\vec{r}) \). We assume that variation of velocity is smooth on the scale of the lattice constant. In this section, we outline the approach used to investigate transport properties through a barrier of velocity and potential.

### 3.1. Current density operator

First, by using the continuity equation, we derive the current density operator. The continuity equation is the following:

\[
\nabla \cdot j = -\partial_t \rho
\]

where \( \rho = \Psi^\dagger \Psi \) is the charge and \( j \) is the current density operator. By using the Schrodinger equation, the divergence of the current density operator is written as

\[
\nabla \cdot j = [(H\Psi)^\dagger \Psi - \Psi^\dagger (H\Psi)]/i\hbar.
\]

By substitution of \( H \) from equation (1) and two component spinors as \( \Psi = (\psi_a, \psi_d)^\dagger \) in the above equation, we have

\[
i\hbar \nabla \cdot j = \left( -i\hbar v_\alpha (\sigma \cdot \nabla) \psi_a + F \psi_d \right)^\dagger \\
\quad \times \left( \psi_a + \left( \psi_a^\dagger + \left( -i\hbar v_\alpha (\sigma \cdot \nabla) \psi_a + \psi_d \right)^\dagger \right) \\
\quad \times \left( -i\hbar v_\delta (\sigma \cdot \nabla) \psi_a + F \psi_d \right)^\dagger \\
\quad \times \left( \psi_a + \left( \psi_a^\dagger + \left( -i\hbar v_\delta (\sigma \cdot \nabla) \psi_a + \psi_d \right)^\dagger \right) \right).
\]

After simplification, it is derived that, interestingly, the current density operator is independent of the gate bias \( \delta \) and also the hopping matrix \( F \).

\[
\nabla \cdot j = [v_\alpha \nabla \cdot (\psi_a^\dagger \sigma^\dagger \psi_a + v_\delta \nabla \cdot (\psi_d^\dagger \sigma_\alpha \psi_d)]
\]

Therefore, the current density operator for a BLG sheet is presented as

\[
j_i = \left( \psi_a \right)^\dagger \left( \begin{array}{cc} v_\alpha \sigma^\dagger & 0 \\ 0 & v_\delta \sigma \end{array} \right) \left( \psi_d \right).
\]

Finally, the current density in the \( i \)th region can be written in the following compact form.

\[
j_i = \Phi_i^\dagger \Sigma \Phi_i
\]

where the auxiliary spinor is defined as \( \Phi_i = \tilde{\psi}_i \Psi_i \) and

\[
\Sigma = \left( \begin{array}{cc} \sigma^\dagger & 0 \\ 0 & \sigma \end{array} \right), \quad \tilde{\psi}_i = \left( \begin{array}{c} \sqrt{v_\alpha} \\ 0 \\ 0 \sqrt{v_\delta} \end{array} \right).
\]

### 3.2. Transfer matrix method

We assume a plane wave solution for the four-band Hamiltonian. So the wavefunction in each region with a constant potential is written as the following matrix product:

\[
\Psi_i(x) = P_i(x) \ast A_i,
\]

where \( P_i(x) \) and \( A_i \) are the plane wave and coefficient matrices, respectively. Details of matrices \( P \) and \( A \) are accessible in appendix B and also in [35, 38]. The local current density in terms of matrices \( P(x) \) and \( A \) in each region reads as follows:

\[
j_i = A_i^\dagger \bar{P}_i^\dagger \Sigma \bar{\psi}_i \bar{P}_i A_i
\]

where the auxiliary spinor in equation (14) has been replaced by \( \Phi_i = \tilde{\psi}_i \Psi_i \). The continuity equation of \( \nabla \cdot j \) \((\vec{r}) = 0 \) leads to the boundary matching condition at interfaces of a junction. In other words, conservation of the current density results in the continuity of the auxiliary spinor \( \Phi_i \) on the boundaries of the barrier junction.

\[
\Phi_1 = \Phi_2 \iff \tilde{\psi}_2 \Psi_2 = \tilde{\psi}_1 \Psi_1.
\]

Referring to the schematic cartoon shown in figure 1, we consider a simultaneous barrier of velocity, and electrostatic potential. At the same time, the barrier can be subjected to a gate bias.

\[
\begin{align*}
\gamma(x) &= \begin{cases} 
\gamma_0 &= \gamma_0(x < 0) \quad \text{III} : x > w \\
\gamma_1 &= \gamma_1(x > w) \quad \text{II} : 0 < x < w
\end{cases} \\
V(x) &= \begin{cases} 
V_0 &= V_0(x < 0) \quad \text{II} : x > w \\
V_0' &= V_0' + \delta/2 \quad \text{II} : 0 < x < w.
\end{cases}
\end{align*}
\]

By applying continuity of the auxiliary spinor on the boundaries of the barrier, one can connect the coefficient matrix related to the last region \( A_3 \) to the coefficient matrix for the first region \( A_1 \).

\[
\begin{align*}
A_1 &= MA_3 \\
M &= P_1^{-1}(0)v_1^{-1}P_2(0)P_3^{-1}(w)v_2^{-1}P_3(0)
\end{align*}
\]

where \( M \) is the transfer matrix. We assume that the energy range of incidence particles in the first region is limited to the range of \( 0 < \varepsilon_1 < t \) [38]. Consequently, the wavenumbers \( \alpha_1^{(1)} \) and \( \alpha_3^{(1)} \), which are defined in appendix B, are real while \( \alpha_1^{(3)} \) and \( \alpha_3^{(3)} \) are imaginary. In this range of energy, coefficient matrices in the first and third regions are proposed in the following form.

\[
A_1 = \left( \begin{array}{cc} 1 & r e_d \\ 0 & 0 \end{array} \right), \quad A_3 = \left( \begin{array}{cc} t & 0 e_d \\ 0 & 0 \end{array} \right)
\]

For the first region, \( e_d \) is the coefficient of the growing evanescent state and \( r \) is the coefficient of reflection. In the last region, \( t \) is the transmission coefficient and \( e_d \) is the coefficient of the decaying evanescent state. By rearrangement of equation (18), the coefficient of transmission is derived as a function of the transfer matrix elements as

\[
t = [M_{11} - M_{13}M_{31}/M_{33}]^{-1}.
\]
The transmission probability of particles through a barrier is defined as the ratio of out-flowing current to in-flowing current.

\[ T = \frac{J_\text{out}}{J_\text{in}} \]  

(20)

where \( J_\text{out} \) is the out-flowing current in the last region and \( J_\text{in} \) is the in-flowing current incidence from the first region. By using equation (15), the transmission probability can be represented in the following form.

\[ T = \frac{\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}. \]  

(21)

The conductance is calculated by using Landauer formalism in the linear regime. Transport is coherent and is calculated at zero temperature. Conductance is proportional to angularly averaged transmission projected along the current direction.

\[ G = 2G_0 \int_0^{\pi/2} T(E, \varphi) \cos(\varphi) \, d\varphi \]  

(22)

where \( G_0 = e^2/mv_F/\hbar^2 \).

### 3.3. Transport across a single velocity barrier

The behavior of a beam produced by Dirac fermions whenever incident on the barrier region is similar to the behavior of an optical beam passing through dielectric materials. In the subsequent sections, we will show that a quantum mechanical version of well known laws in geometrical optics can be also applied to the propagation of Dirac fermions in BLG.

**Case 1.** Let us consider tunneling through a single velocity-induced sharp barrier. For a pure velocity barrier, the types of quasi-particle inside and outside of the barrier are the same for all ranges of energy. For normal incidence \( \theta_1 = 0 \) and in the absence of any gate bias, the transmission coefficient for a velocity barrier with unit velocity ratio \( \eta = 1 \) inside and outside of the barrier can be analytically calculated as

\[ t = e^{i\omega_1 w} \left[ \cos(\alpha_2 w) - iS \sin(\alpha_2 w) \right]^{-1} \]  

(23)

where

\[ S = \frac{1}{2} \left( \alpha_1 \alpha_2 + \frac{\omega_2 \alpha_1}{\omega_1 \alpha_2} \right) \]

and \( \alpha_1 = \sqrt{\omega_1^2 + \omega_1 t/v_1} \) and \( \alpha_2 = \sqrt{\omega_2^2 + \omega_2 t/v_2} \) are the wavevectors along the x-axis direction outside and inside the velocity barrier, respectively. Here, the scaled energy in each region is defined as \( \omega_1 = E/v_1 \) and \( \omega_2 = E/v_2 \).

Replacing defined parameters in \( S \), results in \( S = 1 \). Therefore, transmission probability is derived in the following form:

\[ T = |t|^2 = \frac{1}{\cos^2(\alpha_2 w) + \sin^2(\alpha_2 w)} = 1. \]  

(24)

As a result, for independence of all barrier parameters, transmission at the normal incidence is always perfect. This behavior is similar to what we expect from the standard Klein tunneling. This transparency at the normal incidence will be demonstrated numerically in figure 6. At arbitrary incidence angle, the wavevectors along the x-axis direction in regions I and II can be represented as the following.

\[ \alpha_1 = \sqrt{\frac{1}{v_1^2}(E^2 + tE) - k_y^2}, \]

\[ \alpha_2 = \sqrt{\frac{1}{v_2^2}(E^2 + tE) - k_y^2}. \]  

(25)

Suppose that the velocity outside the barrier \( v_1 \) is set to be \( v_F \). Conservation of the energy \( E \) and the component \( k_y \) of the wavevector across the barrier leads to the following compact form for the wavevector inside the velocity barrier.

\[ \alpha_2 = k - \sqrt{\frac{1}{\xi^2} - \sin^2 \theta_1} \]  

(26)

where \( \xi = \xi_x = \xi_y = v_2/v_1 \) is the velocity of quasi-particles inside the barrier scaled by \( v_F \). \( \theta_1 \) is the incidence angle of quasi-particles which hit the barrier from region I. For the range of \( \xi > 1 \), a look at equation (26) clearly demonstrates that there are some evanescent modes in the barrier region (in which \( \alpha_2 \) is imaginary) if only the incidence angle \( \theta_1 \) is greater than a critical angle, which is defined as

\[ \theta_{cr} = \arcsin(1/\xi). \]  

(27)

In analogy with optics, the total internal reflection (TIR) emerges when a Dirac fermion wave is incident from a denser medium (region I) to a rarer medium (the barrier region II). This behavior is interpreted as \( \xi > 1 \) in our studied system [9, 18, 20–22]. To demonstrate such a critical angle in BLG, we plot transmission probability \( T(\theta_1) \) as a function of incidence angle in figure 6 for several values of velocity. For \( \xi > 1 \) and \( \theta_1 > \theta_{cr} \), transmission is negligible for thick enough barriers. We have also checked that variation of transmission around the critical TIR angle is sharper for the multiple structure of velocity barriers compared with the single velocity barrier. Furthermore, as indicated in figure 6(b), transmission probability shows a sharp change in behavior at \( \xi = 1 \). In the case of \( \eta \neq 1 \), for larger velocity modulated in the upper or lower layer, a smaller critical angle emerges. The critical angle just depends on \( \xi \). So this property is more appropriate for designing a waveguide based on the BLG substrates [20].

As a conclusion for equation (26), for the range of \( \xi < 1 \), the wavevector inside the barrier \( \alpha_2 \) is real, which gives rise to propagating modes. Consequently, some resonance states are expected to emerge. The resonance states obey the
following resonance condition: $\alpha_2(\theta_1, \xi, E)w = n\pi$, where $n$ is the resonant order. As seen in figures 6(a), (b), the velocity barrier is transparent against the propagation of Dirac fermionic waves at the resonance states. The resonance states emerge at special values of the incidence angle, the barrier width and those velocities belonging to the range of $\xi < 1$. To distinguish the propagating from the evanescent modes, we study conductance as a function of barrier width in figure 6(c) for several values of velocity. For $\xi < 1$, the conductance has an oscillatory behavior with the barrier width originating from the propagating modes. On the other hand, the conductance drops sharply to zero for $\xi > 1$, which is an indication of evanescent modes inside the barrier.

3.4. Transport across velocity barrier in presence of a gate bias

Case ii. In this case, the velocity of carriers changes (still $\eta = 1$) in the barrier region, where a perpendicular gate bias is simultaneously applied ($\delta \neq 0$). To clarify transport properties of the mentioned system, it is worthwhile to look at the wavenumber inside the barrier. The wavenumber along the $x$-axis direction is presented as

$$\alpha_2 = k \sqrt{\frac{\mu}{\lambda \xi}} \sin^2 \theta_1$$

Following the procedure of section B.2 gives the critical incidence angle as $\theta_{cr}(E) = \arcsin(\sqrt{\frac{\mu}{\lambda \xi}})$. Note that, in this formula, the critical angle depends on the Fermi energy. Therefore, in the presence of electrostatic gate potentials, this set-up is not proposed as an appropriate material for designing a waveguide. However, a definition of the critical angle for such a system is useful to interpret the behavior of transmission.

A 3D contour plot of transmission in terms of the incidence angle and energy is indicated in figure 7 for two velocity values: (a) $\xi = 1.5$ and (b) $\xi = 0.5$. For $\xi = 1.5$ and for energies greater than the gap $\varepsilon_2 > 0$, the existence of a critical angle is clearly demonstrated in figure 7(a), which shows a sharp drop of transmission to zero. However, such a sharp critical angle is absent for $\xi = 0.5$. As a conclusion, in addition to the parameters $\mu$ and $\lambda$, which are energy dependent, the velocity $\xi$ still can play an important role to tune transporting modes. To manifest such a property, we study conductance as a function of energy in figure 7(c) for $\xi = 0.5$ and 1.5. It is interesting that the conductance for $\xi = 0.5$, is much greater than its value for $\xi = 1.5$. Moreover, the conductance has an oscillatory behavior with the Fermi energy if $\xi < 1$. However, it behaves smoothly with the energy if $\xi > 1$.

Case iii. In the last case, in addition to the gate biasing ($\delta \neq 0$), we modulate the velocities in layers to be not equal to each other, $\eta \neq 1$. Since the band gap of the barrier portion
depends on the velocity ratio $\eta$, we expect to manifest this property by concentrating on the transport gap. Figure 8 represents conductance in terms of energy for several values of the velocity ratio $\eta$. What is novel is that the transport gap appearing in no-transport depends on the velocity ratio $\eta$. The behavior of the conduction and valence band edges with the velocity ratio is in good agreement with those shown in figure 4(c).

Referring to figure 5(a), the dependence of the band gap on the velocity ratio is strong when the gate bias is large, so one can observe that the transport gap depends on the velocity ratio. The transport gap is remarkable when a thick velocity barrier is manipulated in the presence of a large gate bias $\delta$. The maximum band gap emerges at $\eta = 1$.

4. Conclusion

In the presence of a previously applied gate bias, the electronic band structure of bilayer graphene is investigated when quasi-particles have different Fermi velocities in each layer. We address that the velocity engineering is one of the inevitable experimental factors which affects the transport gap in the broken-symmetry BLG.

In the absence of any electrostatic potential, only the modulation of velocity in layers does not cause a band gap.
to open. In other words, the chiral symmetry is conserved for pure velocity modulation $\delta = 0$ while this symmetry will break when a gate bias is subsequently applied on BLG. It should be noted that, in the presence of a gate bias $\delta \neq 0$, the electron–hole symmetry is preserved whenever the same velocity is modulated in both layers; $\eta = 1$. In addition, the band structure keeps its ‘Mexican hat’ shape with a direct band gap. Moreover, the band gap is independent of the velocity value. The maximum value of the band gap occurs at $\eta = 1$. The momentum attributed to the band gap is inversely proportional to the velocity.

In a generic case, non-equal velocities in two layers ($\eta \neq 1$) result in a transition of the direct to indirect band gap. The band gap depends on the velocity ratio $\eta$ and has a peak at $\eta = 1$. Interestingly, the electron–hole symmetry fails; however, the band structure still keeps its ‘Mexican hat’ shape. The shift of momentum from the conduction band edge to the valence band edge is increased with the gate bias.

In the second part, we elaborate a transfer matrix method to calculate coherent tunneling through a velocity barrier possibly subjected to a gate potential. In analogy with optics, we propose a total internal reflection angle $\theta_{cr}$ so that transmission becomes sharply negligible for incidence angles larger than $\theta_{cr}$. The transport gap which is induced by application of the gate bias in the barrier region depends on the velocity ratio.

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Appendix A. The electron–hole asymmetry

To measure the electron–hole (e–h) asymmetry, we define the e–h asymmetric factor as the following: $\langle |E_{c}|/|E_{v}| >$. For the case of equal velocities modulated in both layers $\eta = 1$, the e–h asymmetric factor is zero for the studied Hamiltonian shown in equation (1). However, as seen in figure A.1, this asymmetric factor increases with the momentum much faster than linear behavior [37]. This factor reaches the value of 2 in the special momentum. It is interesting that, by application of the transformation of $\eta \rightarrow 1/\eta$, the e–h asymmetric factor behaves as $r \rightarrow 1/r$.

In addition to the velocity modulation, the e–h asymmetric factor is also originated from the interlayer coupling ($\gamma_{4}$) between $A1–A2$ and $B1–B2$ sites [27, 37]. At the first order approximation, we have not considered such a term in the dominant Hamiltonian shown in equation (1). In fact, the most important terms which affect the main feature of the band structure are $\gamma_{0}$ and $\gamma_{1} = \frac{1}{4} t$. Here, $\gamma_{0}$ is the intra-layer hopping between $A1–B1$ and $A2–B2$ sites, which is proportional to $t_{F}$ in the tight-binding approximation and $\gamma_{1} = \frac{1}{4} t$ is the interlayer coupling between $A2–B1$ sites. The e–h asymmetric factor caused by parameter $\gamma_{4}$ behaves as $4\gamma_{4}/\gamma_{0}$ [27]. The well established values [27] for the hopping parameters are equal to $\gamma_{0} \approx 0.15$ eV and $\gamma_{1} \approx 3$ eV. So the e–h asymmetric factor originating from $\gamma_{4}$ is of the order of magnitude 0.1 [27, 37]. As a conclusion, in the presence of the previously created band gap, the e–h asymmetry arising from the velocity engineering is a dominant factor compared with the e–h asymmetry caused by the parameter $\gamma_{4}$.

Appendix B. Wavefunction

The eigenfunction of the four-band Hamiltonian of equation (1) is defined with the following spinor.

$$\Psi(x) = P(x)A \quad (B.1)$$

where the coefficient matrix is written as

$$A = \begin{pmatrix} U_{A_1} & U_{B_1} & D_{B_1} & D_{A_1} \end{pmatrix}^T$$
and the plane wave matrix is presented as [35, 38]

\[
P(x) = \begin{pmatrix}
  e^{i\alpha_+ x} & e^{-i\alpha_+ x} & e^{i\alpha_- x} & e^{-i\alpha_- x} \\
  f_+^+ e^{i\alpha_+ x} & f_+^- e^{-i\alpha_+ x} & f_-^+ e^{i\alpha_- x} & f_-^- e^{-i\alpha_- x} \\
  s_+^x e^{i\alpha_+ x} & s_+^x e^{-i\alpha_+ x} & s_-^x e^{i\alpha_- x} & s_-^x e^{-i\alpha_- x} \\
  g_+^x s_+^y e^{i\alpha_+ x} & g_+^x s_+^y e^{-i\alpha_+ x} & g_-^x s_-^y e^{i\alpha_- x} & g_-^x s_-^y e^{-i\alpha_- x}
\end{pmatrix}
\]

where \( \alpha_+ \) and \( \alpha_- \) are the wavevectors along the current direction \( (x) \), which is defined as

\[
\alpha_{\pm} = \sqrt{\frac{v_0 (\alpha_{\pm}^2 + k_0^2) \pm \sqrt{a(\epsilon, \eta, \delta)^2 - b(\epsilon, \eta, \delta)^2}}{b(\epsilon, \eta, \delta)}} / v_0.
\]

If the gate voltage turns on, \( a \) and \( b \) defined in equation (2) are functions of \( \epsilon \) instead of \( E \).

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