Bilayer Graphene Interferometry: Phase Jump and Wave Collimation

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We theoretically study the phase of the reflection amplitude of an electron (massive Dirac fermion) at a lateral potential step in Bernal-stacked bilayer graphene. The phase shows anomalous jump of $\pi$, as the electron incidence angle (relative to the normal direction to the step) varies to pass $\pm \pi/4$. The jump is attributed to the Berry phase associated with the pseudospin-1/2 of the electron. This Berry-phase effect is robust against the band gap opening due to the external electric gates generating the step. We propose an interferometry setup in which collimated waves can be generated and tuned. By using the setup, one can identify both the $\pi$ jump and the collimation angle.

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Introduction.— Monolayer graphene has attracted much attention due to potential application of its unusual properties [1]. Its low-energy quasiparticles are massless Dirac fermions. They show Klein tunneling [2], anomalous quantum Hall effects [3, 4], electron optics behavior such as focusing [5] and collimation [6, 7, 8, 9], etc. The Klein tunneling is understood by the chirality of the quasiparticles [2], or equivalently by Berry phase [11, 12]. There have been experimental efforts to observe it in a bipolar junction [12, 13] and in an interferometry [14].

Bilayer graphene has properties quite different from the monolayer. For example, in Bernal-stacked bilayer, low-energy quasiparticles are massive Dirac fermions [15]. There have been studies on bilayer-graphene Klein effects [2], quantum Hall effects [16], band-gap engineering [17, 18, 19, 20], etc. However, more studies on the bilayer may be necessary for the understanding of the features of the massive Dirac fermions such as their transport related with Berry phase [11, 21] and collimation [2].

In this Letter, we theoretically study the reflection of a low-energy electron at a lateral potential step of monopolar $(p-p)$ or $n-n$ type in Bernal-stacked bilayer graphene [Fig. 1(a)]. The phase of the reflection amplitude is found to show anomalous behavior, as the electron incidence angle $\theta_1$ (relative to the normal direction to the step) varies. It shows an abrupt jump of $\pi$ when the step height is much smaller than the kinetic energy of the electron. Based on a reversal symmetry [Eq. (2)], we attribute the jump to the Berry phase associated with the pseudospin-1/2 of the electron. The jump becomes gradual, as the step height increases, due to the evanescent waves existing at the step boundary and breaking the reversal symmetry. We show that the phase jump can be detected in an interferometry setup [Fig. 1(b)]. We remark that the phase jump is robust against the band gap opening due to the electric gates generating the step, and that the setup does not require an external magnetic field, contrary to previous works [2, 11, 14, 16] for the detection of Berry phase effects in graphene.

Potential step.— In Bernal-stacked bilayer graphene, a low-energy electron states $\Psi_K(x, y)$ with energy $E$ in the K valley is governed by Hamiltonian $H_K\Psi_K = E\Psi_K$,

$$H_K = \frac{v^2}{\gamma} \vec{\sigma}_K \cdot \vec{q} + V(x), \quad \vec{q} \equiv (-p_x^2 + p_y^2, -2p_xp_y),$$

(1)

The two pseudospin components of $\Psi_K$ describe the lattice sites $A_1$ and $B_2$ of the bilayer, where $A_1$ and $B_2$ denote the two basis sites of layer $l = 1, 2$. $\vec{\sigma}_K = (\sigma_x, \sigma_y)$ is the pseudospin operator for the K valley, $\vec{p} = (p_x, p_y)$ is the momentum relative to the valley center, $\gamma \approx 0.39$ eV is the interlayer coupling, $v \approx 10^6$ m/s, and $\sigma_{x,y,z}$ are the Pauli matrices. $H_K$ is valid for $0.002\gamma < |E - V| \ll \gamma$, where the trigonal warping is ignored. We study the K valley only, as the K’ valley shows the same result, and ignore the intervalley mixing as $V(x)$ slowly varies on the scales of the lattice constant and $hv/\gamma$. Band gap $\gamma^4$ due to the gates generating $V(x)$ will be considered later.

It is worthwhile to see a symmetry of $H_K$, which has

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.pdf}
\caption{(Color online) (a) Lateral monopolar potential step in Bernal-stacked bilayer graphene ($xy$ plane). The arrows represent the propagation of electron waves, the dashed lines show the boundaries between the regions with different potential strengths $V_i$’s, $\theta_1(\theta_2)$ is the propagation angle of the incident (transmitted) wave, and $r_1$’s ($t_1$’s) are the reflection (transmission) amplitudes. As $\theta_1$ varies, the phase of $r_1$ can exhibit an abrupt jump of $\pi$ at $\theta_1 = \pm \pi/4$, a Berry-phase effect. (b) Interferometry setup for the detection of the $\pi$ phase jump of $r_1$, based on the interference between the two paths drawn in $x \in [0, d_1]$. To see the incidence-angle ($\theta_1$) dependence of $r_1$, collimated waves are generated from a collection of waves with different incidence angle $\theta_{unc}$, by using the resonant filtering due to the barrier $V_c$. The collimation angle $\theta_c$ can be also identified, using the interference.}
\end{figure}
not been discussed in literatures. \(H_K\) is invariant under the antunitary operator \(\Theta\) (for 0.002\(\gamma < |E - V| \ll \gamma\)),

\[
\Theta = i\sigma_y R_{\vec{p}, \pm \pi/2}C,
\]

(2) when \(\vec{p}\) is real (which is achieved when \(V_1 - V_2 \rightarrow 0\) in Fig. 1). Here, \(R_{\vec{p}, \pm \pi/2}\) is the operator rotating \(\vec{p}\) by angle \(\pm \pi/2\) \(|e.c., (p_x, p_y) \rightarrow (\pm p_y, \mp p_x)\) and thus \(\vec{q} \rightarrow -\vec{q}\), \(i\sigma_y C\) reverses pseudospin, and \(C\) is the complex conjugation operator. We call this invariance as reversal symmetry hereafter, in the sense that \(\Theta\) is exactly the same as the time reversal operator defined for a single valley \[22\] if \(\vec{q}\) is replaced by \(\vec{p}\) in Eq. (1). The symmetry \(\Theta\) and the Berry phase \(\pi\) \[23\], associated with a loop encircling once the origin in the \(\vec{q}\) space, can give rise to an interesting effect in a monopolar potential step (see below). This effect corresponds to the Klein tunneling in bipolar monolayer graphene, which results from the time reversal symmetry and the Berry phase \(\pi\) due to a \(\vec{p}\)-space loop \[10, 11\].

Now, we consider a potential step \(V(x)\) of monopolar type, where \(V(x) = V_1\) for \(x < 0\) and \(V_2\) for \(x > 0\), and study the reflection amplitude \(r_1\) of a plane wave incoming to the step with energy \(E\) and incidence angle \(\theta_1\) [Fig. 1(a)], where \(E > V_1, V_2\) (\(E < V_1, V_2\)) for a \(n\) \((p-p)\) step. Due to the translational invariance along \(\vec{y}\), the wave is described by \(\Psi_{K,k_y} = e^{ik_y y} \psi_{K,k_y}(x)\). \(\psi_{K,k_y}(x)\) is a superposition of propagating and evanescent waves \[2\],

\[
e^{ik_{1x}x} \left( e^{-i\theta_1} - e^{-i\theta_1} \right) + r_1 e^{-ik_{1x}x} \left( -e^{i\theta_1} - e^{-i\theta_1} \right)
\]

\[
+ a e^{\kappa_1 x} \frac{\sqrt{1 + \sin^2 \theta_1 + s_1 \sin \theta_1}}{s_1 \sqrt{1 + \sin^2 \theta_1 - \sin \theta_1}} \text{ for } x < 0,
\]

\[
t_1 e^{ik_{2x}x} \left( e^{-i\theta_2} - e^{-i\theta_2} \right)
\]

\[
+ b e^{-\kappa_2 x} \frac{\sqrt{-1 + \sin^2 \theta_2 + s_2 \sin \theta_2}}{-s_2 \sqrt{-1 + \sin^2 \theta_2 - \sin \theta_2}} \text{ for } x > 0.
\]

Here, \(s_j = \text{sgn}(E - V_j),\) \(h_{k_y} = s_1 \sqrt{|E - V_1|/v^2} \sin \theta_1,\)

\(h_{k_{jy}} = s_1 \sqrt{|E - V_1|/v^2} \cos \theta_j,\)

for \(j \in \{1, 2\}\) refers to the region with \(V_j\), and the propagation angle \(\theta_2\) of the transmitted wave is governed by the conservation of \(p_y,\)

\(s_1 \sqrt{|E - V_1|} \sin \theta_1 = s_2 \sqrt{|E - V_2|} \sin \theta_2.\)

The coefficients \(r_1, t_1, a,\) and \(b\) are determined by the continuity of \(\psi_{K,k_y}(x)\) and \(d\psi_{K,k_y}(x)/dx\) at \(x = 0\). We introduce a parameter \(\alpha \equiv (V_2 - V_1)/(E - V_1),\) the ratio of step height and the kinetic energy of the incident wave. The following effects depend only on \(\alpha\) and \(\theta_1\), regardless of other details such as the type \((n-n\) or \(p-p)\) of the step.

Phase jump and Berry phase.— We examine the dependence of the reflection amplitude \(r_1 = |r_1| e^{i\theta_1}\) on \(\alpha\) and \(\theta_1\) \([0, \pi/2]\); \(r_1\) is an even function of \(\theta_1\). We first discuss the case of \(|\alpha| \ll 1\), and then that of finite \(\alpha\).

For \(|\alpha| \ll 1\), the reflection phase \(\theta_\perp\) shows an abrupt jump of \(\pi\) at \(\theta_1 = \pi/4\); see Fig. 2. The phase jump is accompanied by a reflection zero, \(|r_1|^2 = 0\). To see the behavior, we derive the expression of \(r_1\) near \(\theta_1 = \pi/4,

\[
r_1 \simeq \cos 2\theta_1 \alpha \quad \text{for } |\alpha| \ll 1 \text{ and } \theta_1 \simeq \pi/4.
\]

The \(\pi\) jump occurs, irrespective of the sign of \(\alpha\). And, for \(|\alpha| \ll 1\), the evanescent waves are ignorable \((|a|^2, |b|^2 \simeq 0)\), as shown for \(\theta_1 = \pi/4\) in Fig. 3, the same occurs for other values of \(\theta_1\). Below, we attribute the \(\pi\) jump to the Berry phase associated with the pseudospin.

According to the Hamiltonian \[41\], the pseudospin couples with the vector \(\vec{q}\) such that it is parallel (antiparallel) to \(\vec{q}\) in the \(n\)-\((p-p)\) step. We follow the change of \(\vec{q}\) to see the change of the pseudospin in the reflection. The vectors \(\vec{q'}\) of an incident wave \(\Psi_i\) with \(\theta_1 = \pi/4 - \delta\) (where \(\delta\) is a small positive angle) and the wave \(\Psi_f\) formed by the reflection of \(\Psi_i\) at the step are drawn in Fig. 4. One can assign a clockwise path \(\Gamma\) to the change of \(\vec{q}\): the choice between clockwise and counterclockwise does not matter. We also follow the change in the reversal-symmetric process \(\Gamma_{\Theta}\) from \(\Theta\Psi_f\) to \(\Theta\Psi_i\). This process is also a solution of Eq. (1) with the same energy, since the evanescent waves can be ignored and thus \([H_{K}, \Theta] = 0\). Notice that the incidence angle of \(\Theta\Psi_f\) is \(\pi/4 + \delta\), and that \(\Gamma\) and \(\Gamma_{\Theta}\) are reflection-symmetric about \(q_y\) axis. As \(\theta_1 \rightarrow \pi/4\) \((\delta \rightarrow 0)\), the spatial propagation in the process \(\Gamma\) becomes identical to that in \(\Gamma_{\Theta}\). However, at \(\theta_1 = \pi/4\), the change of the pseudospin in the \(\Gamma\) process differs from that in \(\Gamma_{\Theta}\) by \(2\pi\) rotation; i.e., the difference \(\Gamma - \Gamma_{\Theta}\) forms a loop encircling once the origin of the \(\vec{q}\) space.
the dependence of the transmission probability $k$ through the setup on the incidence angle $\theta$. The change from an incident wave $\Psi_i$ (with $\theta_1 < \pi/4$) to its reflected wave $\Psi_f$ is represented by $\Gamma$. The change of the reversal-symmetric process from $\Theta \Psi_f$ (which incidence angle $> \pi/4$) to $\Theta \Psi_i$ is denoted by $\Gamma_{\Theta}$. At $\theta_1 = \pi/4$, $\Psi_i (\Psi_f)$ has the same $\theta$ as $\Psi_f (\Theta \Psi_i)$, but the change of the pseudospin in the process $\Gamma$ differs from that in $\Gamma_{\Theta}$ by 2\pi rotation, resulting in the abrupt $\pi$ jump (Berry phase $\pi$ in the $\hat{q}$ space) of the reflection phase $\theta_{r\Gamma}$.

Berry phase $\pi$ gives rise to the abrupt jump in $\theta_{r\Gamma}$.

We next discuss the case of finite $|\alpha|$. As $|\alpha|$ increases, the abrupt jump of $\theta_{r\Gamma}$ at $\theta_1 = \pi/4$ becomes gradual [Fig. 2]. This is due to the evanescent waves localized at the step boundary $x = 0$, which become to affect the reflection as $|\alpha|$ increases [Fig. 3], and break the reversalsymmetry $\Theta$; for example, a wave $\theta_{i, f}$, $\Psi(\pm ik_{xy}) \propto |k_{xy} \pm i \alpha_0 \hat{y}|$, reversal-symmetric to an evanescent wave $| \pm i \alpha_0 \hat{y}|$, is physically meaningless, as it diverges in $\hat{y}$ direction. For $\theta_1 \simeq \pi/4$ and small $|\alpha|$, we derive

$$\frac{d\theta_{r\Gamma}}{d\theta_1} \simeq \frac{-(\sqrt{3} \alpha/12)}{\left( \theta_1 - \pi/4 + \alpha/4 \right)^2 + (\sqrt{3} \alpha/12)^2} + O(\alpha^3),$$

which shows that the (gradual) jump of $\theta_{r\Gamma}$ occurs around a shifted angle $\theta_1 = (\pi - \alpha)/4$ within $\sqrt{3} |\alpha|/12$. For $|\alpha| > 1$, $\theta_{r\Gamma}$ increases only gradually. Any bipolar step does not show the phase jump, as it has $|\alpha| > 1$.

**Interferometry.**— We propose an interferometry setup for the detection of the phase jump in $\theta_{r\Gamma}$ [Fig. 4(b)]. In addition to the step, it has a potential barrier $V_c$, which shows transmission resonance only around some incidence angle $\theta_c$ [Fig. 4(a)]. This filtering or collimation is used in our setup, to see the dependence of $\theta_{r\Gamma}$ on the incidence angle (now on the collimation angle $\theta_c$).

We first discuss the collimation. Figure 5(a) shows the dependence of the transmission probability $T = |t|^2$ through the setup on the incidence angle $\theta_{unc}$ of a plane wave. Here, $t$ is calculated in the same way as for the step, and we choose $\beta = (V_c - V_1)/(E - V_1) \geq 2$, for which there is no total reflection by the barrier for any $\theta_{unc}$. The collimation angle $\theta_{c\Gamma}$ at which $T$ shows a maximum value for a given $\beta$, is governed by the resonance condition, $2k_{xc \Gamma}d_c + \varphi_0 = 2\pi n (n$ is an integer),

where $k_{xc \Gamma} = s_c k_{in} \sqrt{\beta - 1 - \sin^2 \theta_c}$ is the $\hat{x}$-axis wave vector inside the barrier, $k_{in} = \sqrt{|E - V_1|/\hbar^2}$ is the wave vector of the incident wave, $d_c$ is the barrier width, $s_c = \text{sgn}(E - V_c)$, and $\varphi_0$ is the reflection phase at the barrier boundaries; in our parameter range, the dependence of $\varphi_0$ on $\beta$ and $\theta_{unc}$ is negligible. The collimation is mainly done in the barrier, and negligibly affected by the step, as $|\alpha|$ is small. One can tune $\theta_c$ by changing $\beta$.

Due to the collimation, a wave incoming into the step has incidence angle around $\theta_c$. Its two propagation paths $x \in [0, d_s]$, one with direct transmission and the other with reflection once at $x = d_s$ [Fig. 4(b)], result in the interference pattern of $\cos(2k_{1s}d_s + \theta_{r\Gamma} + \theta_{r\Gamma})$ as a function of $d_s$, where $h k_{1s} = s_1 k_{in} \cos \theta_c$ and $\theta_{r\Gamma}$ is the reflection phase at $x = 0$ [24]; for $\beta \geq 2$, $\theta_{r\Gamma}$ changes only gradually. From the period $\lambda \equiv \pi/k_{1s}$ and the phase shift of the pattern, one can identify $\theta_c$ and the $\pi$ jump of $\theta_{r\Gamma}$.

Based on the above idea, we analyze the conductance $G = (4e^2/h)(W/2\pi) \int dk_y T(k_y)$ through the setup at zero temperature and zero bias, where the factor 4 reflects the spin and valley degeneracy; the integral is done over all the incoming waves with the same energy $E$ but different $\theta_{unc}$, and $W$ is the transverse width of the setup. For different $\beta$’s and thus $\theta_c$’s, the interference pattern in $G$ is shown in Fig. 5(b), as a function of $d_s$. The period of the pattern agrees very well with $\lambda = \pi/k_{1s}$, therefore, from the period, one can identify the collimation angle $\theta_c$ in experiments, provided that $k_{in}$ is known. And, to see the $\pi$ jump of $\theta_{r\Gamma}$, we redraw $G$ in Fig. 5 as a function of $d_s/\lambda$; the jump is not clearly shown in Fig. 5(b), since
dependence of $\xi$ since $0$. and zero temperature, ($\beta$ (0) has to be modified since $H$ by Hamiltonian $\Delta$ $\beta$ $\vec{Q}$ and thus $\delta r$ can be estimated from $\pi/2$ for $\Delta \ll \gamma$ and the argument in Fig. 4 has to be modified since $\beta_0$, one can observe the $\pi$ jump of $\theta_r$.

Discussion.— We include the band gap effect $\Delta(x) = \Delta_1$ due to the external gates creating $V_i$. It is described by Hamiltonian $H_K \simeq H_K + \Delta(x) \sigma_z/2$ for $\Delta \ll \gamma$, and the argument in Fig. 4 has to be modified since $[H_K, \Theta] \neq 0$ for $\Delta \neq 0$. According to Ref. [15], $\Delta_i$ can be expressed, using typical experimental parameters, as $\Delta_i \simeq -2 \xi_i V_i$, where $\xi_i(\epsilon_i) = 0.5(1 + |\epsilon_i|)/[1 + |\epsilon_i| + c_i^2 - 0.5 \ln|\epsilon_i|]$ and $\epsilon_i \equiv V_i/\gamma$. For small $\alpha \equiv (\epsilon_1 - \epsilon_2)/|\epsilon_1|$, we approximately use constant $\xi_{i=1,2} = \xi$, since $\xi_i(\epsilon_i)$ varies slowly enough; we later consider the dependence of $\xi_i$ on $\epsilon_i$. And, in the limit of zero bias and zero temperature, $E \simeq 0$. In this regime of our interest, one can find the unitary pseudospin-rotation $U$ satisfying $UH_KU^\dagger = (s^2/\gamma)\tilde{\sigma}_K \cdot \tilde{Q} + V(x)$, where $\tilde{Q} = (q^2/\gamma)|q|/q^2 + \gamma^2 \Delta_1/(2c_2^2) = \sqrt{1 - \xi^2}$ for all $i$'s. Notice that $UH_KU^\dagger$ has the same form as $H_K$ and that $[UH_KU^\dagger, \Theta] = 0$. Then the argument in Fig. 3 is applicable for $U\Psi_{i,j}$ and $\Theta U\Psi_{i,j}$ in the $\tilde{Q}$ space, thus, the abrupt $\pi$ jump in $\theta_r$ is maintained and can be detected as in Figs. 5 and 4, Eqs. (3)–(4) and Figs. 2 are not altered, and the dependence of $\theta_r$ on $\beta$ is modified slightly. These features persist when we go beyond the approximation made above. For this case of $\xi_1 \neq \xi_2$, Eq. (3) is shifted as $r_1 \rightarrow r_1 + \delta r_1$, where $\delta r_1 \simeq -i\alpha \sin 2\theta_1/(4 \cos^3 \theta_1)$ and $\tilde{Q} = \Delta_1/[2(E - V_1)] - \Delta_2/[2(E - V_2)]$. From $\xi_i(\epsilon_i)$, we find that $\delta r_1$ is ignorable ($|\delta \alpha/\alpha| \lesssim 0.1$) in reasonable ranges of $|\epsilon_i| < 0.2$, $|\alpha| < 0.5$, and $|E/V_2| < 0.2$. This estimation of $\delta r_1$ will be modified only slightly when two (top and bottom) gates are used to create the step with small $V_1 - V_2$; in this general case, the above expression of $\xi_i(\epsilon_i)$ may be altered, but the expression of $\delta r_1$ is still valid. Thus the $\pi$ jump in $\theta_r$ is detectable in the presence of the gap. We emphasize the central role of the $\tilde{Q}$ space as the parameter space for the Berry phase $\pi$.

We compare our result with the Klein effect in monolayer graphene. In the monolayer, it was predicted [13] and observed [14] in an interferometry that a sign change ($\pi$ phase jump) occurs in the back-reflection amplitude. Contrary to our bilayer case, (i) its origin is the Berry phase $\pi$ in the $\vec{q}$ space, (ii) it occurs at zero incidence angle, thus an external magnetic field may be required to detect it, and (iii) it occurs in a bipolar junction.

In summary, we find the abrupt jump $\pi$ of the reflection phase at a monopolar potential step in Bernal-stacked bilayer graphene. The jump is the manifestation of the reversal symmetry $\Theta$ and the Berry phase $\pi$ in the $\vec{Q}$ (or $\vec{q}$) space, and robust against the band gap opening. We propose the setup for the detection of the jump, in which collimated waves are generated, tuned, and identified.

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[23] For bilayer graphene, Berry phase is usually mentioned as $2\pi$ (see, e.g., Ref. [14]), associated with a $\vec{q}$-space loop encircling twice the origin.
[24] We ignore the paths with multiple reflections at $x = d_s$ (as $|r_1|^2 \ll 1$) and those going back to the barrier and re-incoming to the step. They are fully counted in Fig. 5(b).