

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 an anomalous jump of π , 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 π 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 [6–9], etc. The Klein tunneling is understood by the chirality of the quasiparticles [2], or equivalently by Berry phase [10,11]. 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 [15,17–20], 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 [16,21] 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 θ_1 (relative to the normal direction to the step) varies. It shows an abrupt jump of π at $\theta_1 = \pm\pi/4$ when the step height is much smaller than the kinetic energy of the electron. Based on a reversal symmetry [Eq. (2)], we attribute the π 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 [3,4,11,14,16] for the detection of Berry-phase effects in graphene.

Potential step.—In Bernal-stacked bilayer graphene, a low-energy electron state $\Psi_K(x, y)$ with energy E in the K valley is governed by Hamiltonian [15] $H_K\Psi_K = E\Psi_K$,

$$H_K = \frac{v^2}{\gamma} \vec{\sigma}_K \cdot \vec{q} + V(x), \quad \vec{q} \equiv (-p_x^2 + p_y^2, -2p_x p_y). \quad (1)$$

The two pseudospin components of Ψ_K describe the lattice sites A_1 and B_2 of the bilayer, where A_l and B_l 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 [15] 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

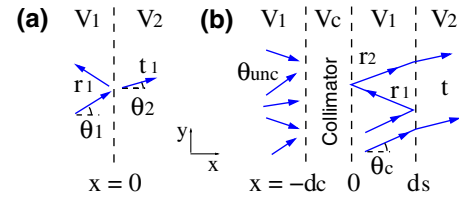


FIG. 1 (color online). (a) Lateral monopolar potential step in Bernal-stacked bilayer graphene (xy plane). The arrows represent the propagation of electron waves, the dashed lines show the boundaries between the regions with different potential strengths V_i 's, $\theta_{1(2)}$ is the propagation angle of the incident (transmitted) wave, and r_i 's (t_i 's) are the reflection (transmission) amplitudes. As θ_1 varies, the phase of r_1 can exhibit an abrupt jump of π at $\theta_1 = \pm\pi/4$, a Berry-phase effect. (b) Interferometry setup for the detection of the π phase jump of r_1 , based on the interference between the two paths drawn in $x \in [0, d_s]$. To see the incidence-angle (here, θ_c) dependence of r_1 , collimated waves are generated from a collection of waves with different incidence angle θ_{unc} , by using the resonant filtering due to the barrier V_c . The collimation angle θ_c can be also identified, using the interference.

the lattice constant and $\hbar v/\gamma$. Band gap [15] due to the gates generating $V(x)$ will be considered later.

It is worthwhile to see a symmetry of H_K , which has not been discussed in the literature. H_K is invariant under the antiunitary operator Θ (for $0.002\gamma < |E - V| \ll \gamma$),

$$\Theta = i\sigma_y \mathcal{R}_{\vec{p}, \pm\pi/2} \mathcal{C}, \quad (2)$$

when $\vec{p}$ is real (which is achieved when $V_1 - V_2 \rightarrow 0$ in Fig. 1). Here, $\mathcal{R}_{\vec{p}, \pm\pi/2}$ is the operator rotating $\vec{p}$ by angle $\pm\pi/2$ [i.e., $(p_x, p_y) \rightarrow (\pm p_y, \mp p_x)$ and thus $\vec{q} \rightarrow -\vec{q}$], $i\sigma_y \mathcal{C}$ reverses pseudospin, and $\mathcal{C}$ is the complex conjugation operator. We call this invariance as reversal symmetry hereafter, in the sense that Θ 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 Θ and the Berry phase π [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 π 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 θ_1 [Fig. 1(a)], where $E > V_1, V_2$ ($E < V_1, V_2$) for a n - n (p - p) step. Because of the translational invariance along $\hat{y}$, 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],

$$\begin{aligned} & e^{ik_{1,x}x} \begin{pmatrix} e^{-i\theta_1} \\ -s_1 e^{i\theta_1} \end{pmatrix} + r_1 e^{-ik_{1,x}x} \begin{pmatrix} -e^{-i\theta_1} \\ s_1 e^{-i\theta_1} \end{pmatrix} + a e^{\kappa_{1,x}x} \begin{pmatrix} \sqrt{1 + \sin^2\theta_1} + s_1 \sin\theta_1 \\ s_1 \sqrt{1 + \sin^2\theta_1} - \sin\theta_1 \end{pmatrix} \quad \text{for } x < 0, \\ & t_1 e^{ik_{2,x}x} \begin{pmatrix} e^{-i\theta_2} \\ -s_2 e^{i\theta_2} \end{pmatrix} + b e^{-\kappa_{2,x}x} \begin{pmatrix} -\sqrt{1 + \sin^2\theta_2} + s_2 \sin\theta_2 \\ -s_2 \sqrt{1 + \sin^2\theta_2} - \sin\theta_2 \end{pmatrix} \quad \text{for } x > 0. \end{aligned}$$

Here, $s_j = \text{sgn}(E - V_j)$, $\hbar k_{j,y} = s_1 \sqrt{|E - V_1| \gamma / v^2} \sin\theta_1$, $\hbar k_{j,x} = s_j \sqrt{|E - V_j| \gamma / v^2} \cos\theta_j$, $\hbar \kappa_j = \sqrt{|E - V_j| \gamma / v^2} \times \sqrt{1 + \sin^2\theta_j}$, $j \in \{1, 2\}$ refers to the region with V_j , and the propagation angle θ_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 α and θ_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 $r_1 = |r_1| e^{i\theta_{r_1}}$ on α and $\theta_1 \in [0, \pi/2]$; r_1 is an even function of θ_1 . We first discuss the case of $|\alpha| \ll 1$, and then that of finite α .

For $|\alpha| \ll 1$, the reflection phase θ_{r_1} shows an abrupt jump of π 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 $\theta_1 = \pi/4$,

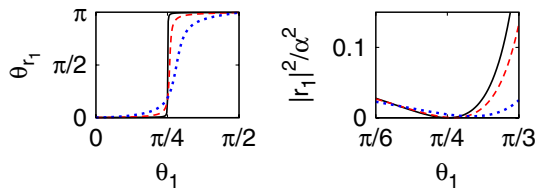


FIG. 2 (color online). Dependence of the reflection phase θ_{r_1} and probability $|r_1|^2$ (scaled by α^2) on θ_1 for $\alpha = -0.01$ (solid), -0.1 (dashed), and -0.5 (dotted). Around $\theta_1 = \pi/4$, θ_{r_1} shows a jump of π , accompanied by $|r_1|^2 = 0$.

$$r_1 \simeq -\frac{\cos 2\theta_1}{4\cos^2\theta_1} \alpha \quad \text{for } |\alpha| \ll 1 \quad \text{and} \quad \theta_1 \simeq \pi/4. \quad (3)$$

The π jump occurs, irrespective of the sign of α . 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 θ_1 . Below, we attribute the π jump to the Berry phase associated with the pseudospin.

According to the Hamiltonian (1), the pseudospin couples with the vector $\vec{q}$ such that it is parallel (antiparallel) to $\vec{q}$ in the n - 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 Ψ_i with $\theta_1 = \pi/4 - \delta$ (where δ is a small positive angle) and the wave Ψ_f formed by the reflection of Ψ_i at the step are drawn in Fig. 4. One can assign a clockwise path Γ 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 Γ_Θ 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 Γ and Γ_Θ are reflection-symmetric about q_y axis. As $\theta_1 \rightarrow \pi/4$ ($\delta \rightarrow 0$), the spatial propagation in the process Γ becomes iden-

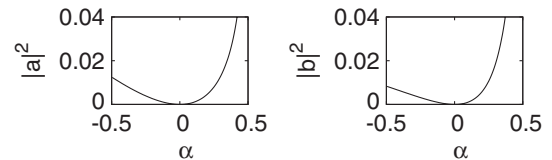


FIG. 3. Dependence of the probabilities $|a|^2$ and $|b|^2$ of the evanescent waves on α at $\theta_1 = \pi/4$.

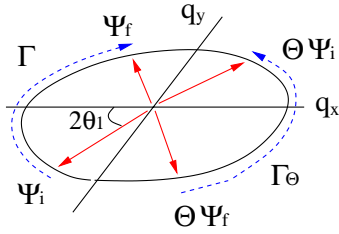


FIG. 4 (color online). Schematic view of the change of $\vec{q}$ in the reflection process for $|\alpha| \ll 1$. This view also shows the change of pseudospin, since pseudospin is parallel (antiparallel) to $\vec{q}$ in the n - n (p - p) step. The change from an incident wave Ψ_i (with $\theta_1 < \pi/4$) to its reflected wave Ψ_f is represented by Γ . The change of the reversal-symmetric process from $\Theta\Psi_f$ (which incidence angle $> \pi/4$) to $\Theta\Psi_i$ is denoted by Γ_Θ . At $\theta_1 = \pi/4$, Ψ_i (Ψ_f) has the same $\vec{q}$ as $\Theta\Psi_f$ ($\Theta\Psi_i$), but the change of the pseudospin in the process Γ differs from that in Γ_Θ by 2π rotation, resulting in the abrupt π jump (Berry phase π in the $\vec{q}$ space) of the reflection phase θ_{r_1} .

tical to that in Γ_Θ . However, at $\theta_1 = \pi/4$, the change of the pseudospin in the Γ process differs from that in Γ_Θ by 2π rotation, i.e., the difference $\Gamma - \Gamma_\Theta$ forms a loop encircling once the origin of the $\vec{q}$ space. The resulting Berry phase π gives rise to the abrupt jump in θ_{r_1} .

We next discuss the case of finite α . As $|\alpha|$ increases, the abrupt jump of θ_{r_1} 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 reversal symmetry Θ ; for example, a wave $\Theta|\pm i\kappa_j, k_y\rangle \propto |k_y, \pm i\kappa_j\rangle$, reversal symmetric to an evanescent wave $|\pm i\kappa_j, k_y\rangle$, is physically meaningless, as it diverges in $\hat{y}$ direction. For $\theta_1 \simeq \pi/4$ and small $|\alpha|$, we derive

$$\frac{d\theta_{r_1}}{d\theta_1} \simeq \frac{-(\sqrt{3}\alpha/12)}{(\theta_1 - \pi/4 + \alpha/4)^2 + (\sqrt{3}\alpha/12)^2} + O(\alpha^3), \quad (4)$$

which shows that the (gradual) jump of θ_{r_1} occurs around a shifted angle $\theta_1 = (\pi - \alpha)/4$ within $\sqrt{3}|\alpha|/12$. For $|\alpha| \geq 1$, θ_{r_1} increases only gradually. Any bipolar step does not show the phase jump, as it has $|\alpha| \geq 1$.

Interferometry.—We propose an interferometry setup for the detection of the phase jump in θ_{r_1} [Fig. 1(b)]. In addition to the step, it has a potential barrier V_c , which shows transmission resonance only around some incidence angle θ_c [Fig. 5(a)]. This filtering or collimation [2] is used in our setup, to see the dependence of θ_{r_1} on the incidence angle (now on the collimation angle θ_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 θ_{unc} of a plane wave. Here, t is calculated in the same way as for the step, and we choose $\beta \equiv (V_c - V_1)/(E - V_1) \geq 2$, for which there is no total reflection by the barrier for any θ_{unc} . The collimation angle θ_c , at which T shows a maximum value for a given β , is governed by the resonance condition,

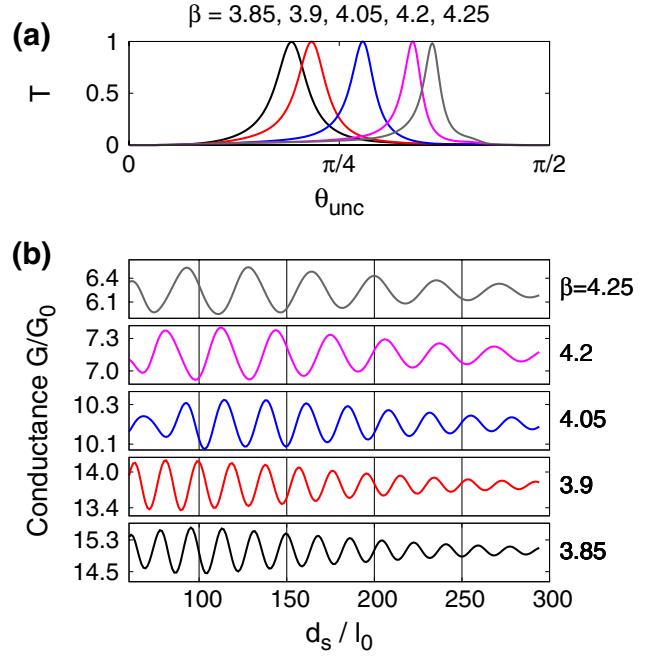


FIG. 5 (color online). (a) Transmission $T = |t|^2$ of a plane wave with incidence angle θ_{unc} through the setup in Fig. 1(b), for different β 's. T is an even function of θ_{unc} . (b) Conductance G as a function of d_s . In (a) and (b), $E - V_1 = 0.04\gamma$, $\alpha = -0.5$, and $d_c = 60l_0$ are chosen, while $d_s = 60l_0$ only in (a). Here, $G_0 \equiv e^2W/(2\pi\hbar d_c)$ and $l_0 \equiv \hbar v/\gamma \approx 1.7$ nm.

$2k_{c_x}d_c + \varphi_0 = 2\pi n$ (n is an integer), where $k_{c_x} = s_c k_{\text{in}} \sqrt{|\beta - 1| - \sin^2\theta_c}$ is the $\hat{x}$ -axis wave vector inside the barrier, $k_{\text{in}} = \sqrt{|E - V_1|\gamma/(\hbar v)^2}$ is the wave vector of the incident wave, d_c is the barrier width, $s_c = \text{sgn}(E - V_c)$, and φ_0 is the reflection phase at the barrier boundaries; in our parameter range, the dependence of φ_0 on β and θ_{unc} is ignorable. The collimation is mainly done in the barrier, and negligibly affected by the step, as $|r_1|$ is small. One can tune θ_c by changing β .

Because of the collimation, a wave incoming into the step has incidence angle around θ_c . Its two propagation paths in $x \in [0, d_s]$, one with direct transmission and the other with reflection once at $x = d_s$ [Fig. 1(b)], result in the interference pattern of $\cos(2k_{1_x}d_s + \theta_{r_1} + \theta_{r_2})$ as a function of d_s , where $\hbar k_{1_x} = s_1 k_{\text{in}} \cos\theta_c$ and θ_{r_2} is the reflection phase at $x = 0$ [24]; for $\beta \geq 2$, θ_{r_2} changes only gradually. From the period $\lambda \equiv \pi/k_{1_x}$ and the phase shift of the pattern, one can identify θ_c and the π jump of θ_{r_1} .

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 θ_{unc} , and W is the transverse width of the setup. For different β 's and thus θ_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 $\lambda = \pi/k_{1_x}$, therefore, from the

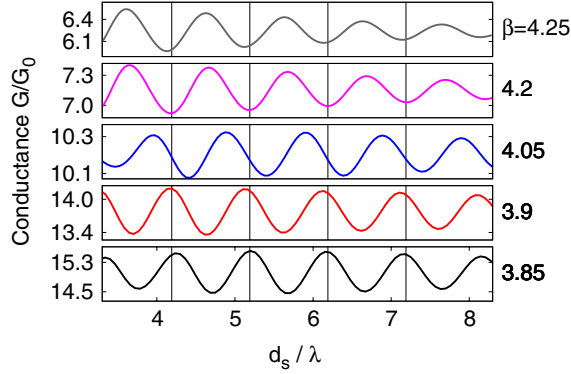


FIG. 6 (color online). The same as in Fig. 5(b), but as a function of d_s/λ .

period, one can identify the collimation angle θ_c in experiments, provided that k_{in} is known. And, to see the π jump of θ_{r_1} , we redraw G in Fig. 6, as a function of d_s/λ ; the jump is not clearly shown in Fig. 5(b), since λ varies with β . It shows the phase shift by π around $\beta = 4.05$, where $\theta_c = 1.11\pi/4$; the value $1.11\pi/4$ deviates from $\pi/4$, and the deviation roughly agrees with the deviation $\alpha/4$ for small α [see Eq. (4)]. In this way, by tuning β and thus θ_c , one can observe the π jump of θ_{r_1} .

Discussion.—We include the band-gap effect $\Delta(x) = \Delta_i$ 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], Δ_i can be expressed, using typical experimental parameters, as $\Delta_i \simeq -2\xi_i V_i$, where $\xi_i(\epsilon_i) = 0.5(1 + |\epsilon_i|)/[1 + |\epsilon_i| + \epsilon_i^2 - 0.5 \ln|\epsilon_i|]$ and $\epsilon_i \equiv V_i/\gamma$. For small $\alpha \simeq (\epsilon_1 - \epsilon_2)/\epsilon_1$, we approximately use constant $\xi_{i=1,2} = \xi$, since $\xi_i(\epsilon_i)$ varies slowly enough; we later consider the dependence of ξ_i on ϵ_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 $UH'_K U^\dagger = (v^2/\gamma)\vec{\sigma}_K \cdot \vec{Q} + V(x)$, where $\vec{Q} \equiv (\vec{q}/|\vec{q}|)\sqrt{q^2 + \gamma^2\Delta_i^2/(2v^2)^2} = \vec{q}/\sqrt{1 - \xi^2}$ for all i 's. Notice that $UH'_K U^\dagger$ has the same form as H_K and that $[UH'_K U^\dagger, \Theta] = 0$. Then the argument in Fig. 4 is applicable for $U\Psi_{i,f}$ and $\Theta U\Psi_{i,f}$ in the $\vec{Q}$ space, thus, the abrupt π jump in θ_{r_1} is maintained and can be detected as in Figs. 5 and 6; Eqs. (3) and (4) and Figs. 2 and 3 are not altered, and the dependence of θ_c on β 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 $\delta r_1 \simeq -i\tilde{\alpha} \sin 2\theta_1/(4\cos^2\theta_1)$ and $\tilde{\alpha} = \Delta_1/[2(E - V_1)] - \Delta_2/[2(E - V_2)]$. From $\xi_i(\epsilon_i)$, we find that δr_1 is ignorable ($|\tilde{\alpha}/\alpha| \lesssim 0.1$) in reasonable ranges of $|\epsilon_i| < 0.2$, $|\alpha| < 0.5$, and $|E/V_2| < 0.2$. This estimation of δr_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 δr_1

is still valid. Thus the π jump in θ_{r_1} is detectable in the presence of the gap. We emphasize the central role of the $\vec{Q}$ space as the parameter space for the Berry phase π .

We compare our result with the Klein effect in monolayer graphene. In the monolayer, it was predicted [11] and observed [14] in an interferometry that a sign change (π phase jump) occurs in the back-reflection amplitude. Contrary to our bilayer case, (i) its origin is the Berry phase π in the $\vec{p}$ 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 π of the reflection phase at a monopolar potential step in Bernal-stacked bilayer graphene. The jump is the manifestation of the reversal symmetry Θ and the Berry phase π 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 2π (see, e.g., Ref. [16]), 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-incident to the step. They are fully counted in Fig. 5(b).