Electronic topological transition in sliding bilayer graphene

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We demonstrate theoretically that the topology of energy bands and Fermi surface in bilayer graphene undergoes a very sensitive transition when an extremely tiny lateral interlayer shift occurs in arbitrary directions. The phenomenon originates from a generation of an effective non-Abelian vector potential in the Dirac Hamiltonian by the sliding motions. The characteristics of the transition such as pair annihilations of massless Dirac fermions are dictated by the sliding direction owing to a unique interplay between the effective non-Abelian gauge fields and Berry’s phases associated with massless electrons. The transition manifests itself in various measurable quantities such as anomalous density of states, minimal conductivity, and distinct Landau level spectrum.

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I. INTRODUCTION

Changes in the topology of Fermi surfaces known as Lifshitz transition alter physical properties of metals significantly. Though such an electronic topological transition (ETT) has been pursued in various materials, its realization requires large external perturbations such as alloying or applying high pressure that hinder clear detections of the transition. Recent progress in measuring low energy electronic structures of bilayer graphene (BLG) provides a new opportunity to explore the ETT because of its unique electronic structures and because of the possible noninvasive control of chemical potential of the system.

In BLG, two coupled hexagonal lattices of carbon atoms are arranged according to Bernal stacking. Because BLG has a large degeneracy at the charge neutral point, there have been intense discussions on possible many-body effects in the system. Moreover, since electrons in a single layer graphene (SLG) behave as relativistic massless fermions, BLG provides a unique playground to control interactions between relativistic particles coupled with the relative mechanical motions of two layers. Hence, the effects of rotational stacking fault on physical properties of BLG have been studied extensively; however, the effect of sliding one layer with respect to the other has not. This mechanical motion is important because the interactions between the two layers are sensitive to the deviation from Bernal stacking and extremely small sliding will change its low energy electronic structures significantly.

In this paper, we predict a very sensitive topological change in the energy bands and Fermi surfaces of BLG when sliding motion or interlayer shear occurs. It is demonstrated that a peculiar coupling between the effective gauge potential with SU(4) symmetry generated by sliding motions and Berry’s phase of massless Dirac fermions play a crucial role to change the topology of low energy bands of BLG. It gives rise to either pair annihilations of massless Dirac fermions or generations of fermions by absorbing fermions with topological charges, depending on sliding directions. This will offer new opportunities to realize the ETT driven by non-Abelian gauge fields with gentle maneuverable mechanical operations.

We start with a detailed description of our first-principles calculation methods including a correction for interlayer dispersive forces. The energetics and changes of the interlayer distance for sliding BLG are presented also. Then, the low energy electronic structures obtained by the calculation are discussed when BLG experiences very small sliding between the two layers. The next three sections introduce a model Hamiltonian for the system and discuss the role of gauge potential and Berry’s phase for the changes in low energy electronic structures. Several spectroscopic consequences will be discussed in the final section.

II. FIRST-PRINCIPLES CALCULATION METHODS AND ATOMIC STRUCTURES

Our electronic structure calculation employs the first-principles self-consistent pseudopotential method using the generalized gradient approximation (GGA) for exchange-correlation functional complemented by Perdew, Burke, and Ernzerhof (PBE). A kinetic energy cutoff for wavefunction of 65 Rydberg is employed and a plane-wave basis set is used. The ion core of carbon atom is described by ultrasoft pseudopotentials. A k-point sampling of 60 × 60 × 1 k points uniformly distributed in the two-dimensional Brillouin zone (BZ) is used in self-consistent calculations and 150 × 150 × 1 k points is sampled to obtain electronic energy bands on a rectangular grid of 1.2% of the first BZ size around the K-point. Since we have dealt with sub-Angstrom displacements of atoms, we have tested our calculation as increasing the cutoff to 120 Rydberg (corresponding to a kinetic energy cutoff of 480 Rydberg for charge density and potential) finding no differences in results. The total charge was calculated by using the Marzari-Vanderbilt cold smear-
and inter-layer hopping parameter, the bottom layer slides with respect to the top layer 1 by $d_x\delta_i$. In the top, $\delta_2 = (0, -1)a_c$, $\delta_2 = (-\frac{\sqrt{3}}{2}, \frac{1}{2})a_c$, and $\delta_3 = (\frac{\sqrt{3}}{2}, \frac{1}{2})a_c$. (b) Schematic diagrams for stacking under various sliding directions. (c) The $nn$ intra- and inter-layer hopping parameter, $-\gamma_0$ and $-\gamma_1$. (d) The $nnn$ inter-layer hopping (between $B_1-A_2$, $-\gamma_3$ with sliding. (e) The smallest inter-layer hopping (between $A_1-A_2$ or $B_1-B_2$), $-\gamma_4$ with sliding.

Since the GGA cannot describe the interlayer interaction between graphene properly, we have employed a semiemirical function of van der Waals (vdW) forces to our calculations following Grimme’s proposal. Within the semiemirical method, the total energy of the system is $\mathcal{E}_{\text{PBE+vdW}} = \mathcal{E}_{\text{PBE}} + \mathcal{E}_{\text{vdW}}$ where $\mathcal{E}_{\text{PBE}}$ is the total energy from GGA functional of PBE and the total energy given by dispersive forces is $\mathcal{E}_{\text{vdW}}$ which can be written as $\mathcal{E}_{\text{vdW}} = -\frac{1}{2} \sum_{ij} C_{ij} \sum_i \sum_j f_{\text{damp}} (|\vec{r}_{ij} + \vec{R}|)|\vec{r}_{ij} + \vec{R}|^{-6}$, where $f_{\text{damp}} = s_6 \cdot (1 + e^{-d (|\vec{r}_{ij} + \vec{R}|/r_0-1)})^{-1}$, $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$ is a vector for carbon-carbon distance, $\vec{R}$ a lattice vector, $s_6$ a scaling parameter, and $d$ a damping parameter, respectively.

The coefficient of dispersive forces of $C_{ij}$ and a sum of vdW radii $r_0$ are computed for each pair of atoms $i$ and $j$ such that $C_{\delta_{ij}} = \sqrt{C_{6\delta_{ij}}}$ and $r_0 = r_{00} + r_{0j}$. We have used $C_6 = 1.75 \text{ J nm}^6 \text{ mol}^{-1}$ and $r_0 = 1.451 \text{ Å}$ for carbon atom suggested by Grimme and $d = 20$, $s_6 = 0.65$ for our GGA calculations. Here, $i$ and $j$ for $\mathcal{E}_{\text{vdW}}$ run through all atoms in the unit cell and $\vec{R}$ satisfies a criteria of $|\vec{r}_{ij} + \vec{R}| < 100\text{ Å}$. Atomic structures of sliding BLG are shown in Figs. 1(a) and 1(b). Without sliding, carbon atoms in BLG are arranged according to Bernal stacking - carbon atoms in one sublattice of the upper layer are right on top of ones in the other sublattice of the lower layer. When the bottom layer slides with respect to the top layer, the sliding vector $\vec{d}_s$ can be written as a linear combination of $\vec{d}_i$ ($i = 1, 2, 3$) which connect the nearest neighbor ($nn$) carbon atoms in the top layer (For definitions of $\delta_i$ ($i = 1, 2, 3$), see Fig. 1). Considering the lattice structures of sliding bilayer, it is easy to check that the sliding along $\pm \delta_1$ is equivalent to one along $\pm \delta_1(3)$. We also note that a sliding along $\delta_3$ is equivalent to one along $-\delta_1$. Full sliding along $\delta_1$ brings an AB-stacking bilayer graphene to a BA-stacking bilayer graphene while one along $\delta_3$ shifts an AB-stacking bilayer to a AA-stacking bilayer.

We find that the equilibrium interlayer distance of bilayer graphene (BLG) in Bernal stacking is 3.348 Å and its binding energy is 38.76 meV (Fig. 2 (a)), which are in good agreement with other calculations and available experimental data. When bilayer graphene has AA-stacking (one layer is right on top of the other layer), the interlayer distance increases to 3.635 Å and binding energy decreases to 30.77 meV (Fig. 2 (b)). When one graphene layer slides with respect to the other along either $\delta_1$ or $\delta_3$ direction, the binding energy starts decreasing and interlayer distance increases agreeing with a previous study. We note that the change in the binding energy ($< 0.19$ meV) and interlayer distance ($< 0.01$ Å) is quite negligible when the sliding distance is less than 0.14 Å (about 10 % of the
III. LOW ENERGY BAND STRUCTURES FROM GGA CALCULATIONS

Considering the low energy electronic structure of BLG in Bernal stacking, our calculations show, as in a previous study, four Dirac cones formed around the Fermi energy ($E_F$) at four Dirac points ($k_{D_i}$, $i = 0, 1, 2, 3$) near around $K$-point [Fig. 3(a) and 3(b)]. The magnitude of $k_{D_i}$ ($i = 1, 2, 3$) is about 0.4% of the distance between Gamma point ($\Gamma$) to $K$-point ($\Gamma K$) [Fig. 3(b)]. As the energy moves away from the $E_F$, the four Dirac cones merge to form three saddle points between the cones [Fig. 3(b)]. The calculation result can also be described by an effective Hamiltonian,

$$H_{\text{eff}}(\vec{k}) = \hbar v_\alpha \vec{\tau} \cdot \vec{k} + \frac{\hbar^2 v_0^2}{\gamma_1} (\vec{\tau} \cdot \vec{k}) \tau_x(\vec{\tau}^* \cdot \vec{k}),$$

(1)

where $v_\alpha = (3/2)\gamma_0 a_c/\hbar$ ($\alpha = 0, 3$), $h\vec{k} = h(k_x, k_y)$ is the crystal momentum from $K$-point, and $\vec{\tau} = (\tau_x, \tau_y)$ and $\vec{\tau}^*$ are Pauli spin matrices and their complex conjugates (See Fig. 1 for definition of $\gamma_\alpha$). Typical estimates are $\gamma_0 \simeq 3$ eV, $\gamma_1 \simeq \gamma_3 \simeq \gamma_0/10$ and $\gamma_4 \simeq \gamma_0/20$ (Ref.36). We will neglect $\gamma_4$ and discuss its role in Sec. VI. If we expand the effective Hamiltonian around each $k_{D_i}$, we have one isotropic Dirac Hamiltonian, $H_{D0} = \hbar v_3 \vec{\tau} \cdot \vec{k}_0$ at $k_{D0}$, an anisotropic $H_{D1} = \hbar v_3 (\vec{\tau} \cdot \vec{\tau}_D x + 3\gamma_1^0 \vec{\tau} \cdot \vec{k}_y)$ at $k_{D1}$, and two anisotropic others at $k_{D2}$ and $k_{D3}$ which can be obtained by rotating $H_{D1}$ by $\pm 2\pi/3$ respectively. Here, $\delta k_i = (\delta k_{x1}, \delta k_{y1}) = \vec{k} - k_{D1}, (i = 0, 1, 2, 3)$.

We find that the low energy bands of BLG change dramatically when one layer slides with respect to the other in an extremely small amount and in arbitrary directions. Let the bottom layer slide with respect to the top by $d_s = (d_x, d_y)$ [Fig. 1(a) and 1(b)]. First, when the bottom layer moves along $\delta_1$ direction by 0.028 Å, i.e., $d_s = 0.02\delta_1$, only two Dirac cones at $k_{D2}$ and $k_{D3}$ remain, instead of four cones for BLG without sliding as shown in Fig. 3(c). The energetic position of the saddle points of the valence band decreases from $-1.1 \text{ meV}$ to $-7.2 \text{ meV}$. When the bottom layer slides further ($d_s = 0.1\delta_1$), the topological changes again and the saddle point energy significantly decreases to $-32.7 \text{ meV}$ [Fig. 3(d)]. Second, when the bottom layer moves along the direction opposite to the previous one ($d_s = -0.02\delta_1$), the low energy bands change again completely. In this case, the Dirac cone at $k_{D1}$ moves along the $-k_x$ direction and an anomalous Dirac cone with sickle-shaped energy contours appears at a new Dirac point instead of three cones [Fig. 3(e)]. If the bottom layer slides further by 0.14 Å along $-\delta_1$ ($d_s = -0.1\delta_1$), the topology remains the same and the anomalous cone comes to have an anisotropic shape [Fig. 3(f)]. In this case, the saddle point energy decreases to $-48.5 \text{ meV}$ (almost 500% of pristine one) [Fig. 3(f)]. Finally, when we slide the bottom layer by 0.012($\delta_3 - \delta_1$) [Fig. 3(g)] and 0.1($\delta_3 - \delta_1$) [Fig. 3(h)], the topological changes are similar to the case for the sliding along $-\delta_2$. The saddle point energy for the sliding by 0.1($\delta_3 - \delta_1$) decreases dramatically down to $-74.0 \text{ meV}$ as shown in Fig. 3(h). After a comprehensive search for the topological changes by the sliding along arbitrary directions (not shown here), we find that the topology of saddle point energy contours is all similar to those shown in Fig. 3(e)-(h).
(one crossing point) except the topologically distinctive phase in Fig. 3(c) (two crossing points).

IV. EFFECTIVE MODEL HAMILTONIANS AND NON-ABELIAN GAUGE POTENTIAL

The hypersensitive topological changes found by first-principles calculations in the previous section demonstrate that the sliding motion creates interactions between the effective non-Abelian SU(4) gauge field background and massless fermions. In the presence of a very tiny sliding, the nnn interlayer interaction ($\gamma_3$) is not constant any more but depends exponentially on the different pair distances between carbon atoms in top and bottom layers as shown in Fig. 1(d). The asymmetric inter-layer hopping interaction produces a constant pseudo-gauge potential in the terms of Hamiltonian containing $\gamma_3$ only, being similar with an effective Hamiltonian for strained SLG\textsuperscript{37–40}. Hence, the effective Hamiltonian for sliding BLG can be written as,

$$H_{\text{eff}}(\vec{k}) = \hbar v_3 \vec{\tau} \cdot (\vec{k} - \vec{\lambda}) + \frac{\hbar v_3}{p_D} (\vec{\tau}^x \cdot \vec{k}) \tau_x (\vec{\tau}^x \cdot \vec{k})$$

(2)

where $p_D \equiv \gamma_1 v_3/(\hbar v_0^3)$ and $\gamma_1$ is the reduced nn interlayer interaction. (See Appendix for derivation of Eq. (2).) We find that the constant vector potential ($\vec{\lambda}$) explicitly depends on the sliding vector, $\vec{\lambda} \equiv (\lambda_x, \lambda_y, \lambda_z) = \beta (d_{xy} - d_{xz})$. By fitting the energy bands obtained by the model to ones by the first-principles calculation, we can estimate that $\beta$ is about $1/a_c^2$. The gauge symmetry in Eq. (2) apparently seems to be broken since $\vec{\lambda}$ is absent in the quadratic term of $\vec{k}$. However, when we expand Eq. (1) at each Dirac point ($\vec{k}_{Di}$), the four Dirac cones shift depending on both $\vec{\lambda}$ and their own positions as $\vec{k}_{Di} \rightarrow \vec{k}_{Di} + \vec{A}_i(\vec{k})$ ($i = 0, 1, 2, 3$). If $|\vec{\lambda}| \ll p_D$, $\vec{A}_0 = (\lambda_x, \lambda_y, 0)$, $\vec{A}_1 = (-\lambda_x, \frac{\lambda_y}{\sqrt{2}}, 0)$, $\vec{A}_2 = (\frac{\lambda_x}{\sqrt{2}}, -\frac{\lambda_y}{\sqrt{2}}, -2\lambda_z)$ and $\vec{A}_3 = (\frac{\lambda_x}{\sqrt{2}}, \frac{\lambda_y}{\sqrt{2}}, -\frac{2\lambda_z}{3})$. So, each Dirac cone moves along a different direction depending on its position.

The essential feature of the system that enables the electronic topological transition in BLG is the shift of four Dirac points along different directions under the sliding of one layer against the other. As we have shown, the effect of sliding is to replace $\delta k_i = \vec{k} - \vec{k}_{Di}$ with $\delta k_i - \vec{A}_i$ in the effective Hamiltonian for the low energy modes near the Dirac points and this feature suggests that the sliding in BLG induces a non-Abelian background gauge field associated with these modes. In order to show this more explicitly, we assume that before sliding, there are four massless Dirac fermions, labeled by $i = 0, 1, 2, 3$, whose Hamiltonians are all isotropic and of same chirality:

$$H_{Di} = \hbar v_3 \vec{\tau}^x \cdot \delta k_i, \quad i = 0, \ldots, 3.$$

(3)

We can then form a quadruplet out of four fermions, so that the index $i$ is now viewed as the “color” index of SU(4) symmetry, and combine the four Hamiltonians $H_{Di}$ compactly as $H_D = \hbar v_3 (\vec{\tau}^x \cdot \delta \vec{k}) \otimes I$, where $I$ is the 4x4 identity matrix. If we now introduce the background gauge field $\vec{A} = (A_x, A_y)$ for the SU(4) symmetry with

$$A_x = \lambda_x \left[ \begin{array}{ccc} 1 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & -1 \end{array} \right],$$

and

$$A_y = \frac{\lambda_y}{\sqrt{3}} \left[ \begin{array}{ccc} 0 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{array} \right] + \lambda_y \left[ \begin{array}{ccc} 1 & -2 & 0 \\ \frac{1}{3} & -\frac{2}{3} & 0 \\ 0 & 0 & -2 \end{array} \right],$$

so that $\delta \vec{k} I \rightarrow \delta \vec{k} I - \vec{A}$ in the Hamiltonian, then Eq. (3) now becomes

$$H_{Di} = \hbar v_3 \vec{\tau}^x \cdot (\delta \vec{k}_i - \vec{A}_i), \quad i = 0, \ldots, 3,$$

(4)

where $\vec{A}_i$ are precisely the shifts of the Dirac points shown at the beginning of this section. Since both $A_x$ and $A_y$ are linear combinations of the generators of SU(4), we now see the effect of sliding as if introducing a non-Abelian background gauge field.

The low energy Hamiltonian of bilayer graphene is different from what we have just shown above in that $H_{D0}$ has opposite chirality from $H_{Di}$ for $i = 1, 2, 3$, and that the latter three Hamiltonians are anisotropic. A parity inversion $\delta k_y \rightarrow -\delta k_y$ for $H_{D0}$ and anisotropic rescalings of $\delta k_i$ for $H_{Di}$ ($i = 1, 2, 3$) transform SU(4) isotropic quadruplet to the low energy Hamiltonian of BLG. This transformation is equivalent to multiplying the Pauli matrices $\tau_x$ and $\tau_y$ with (different) constants in Eq. (4) — for example, $(\tau_x, \tau_y) \rightarrow (-\tau_x, -\tau_y)$ for $i = 0$, and $(\tau_x, \tau_y) \rightarrow -(\tau_x, 3\tau_y)$ for $i = 1$ — thereby breaking the SU(4) symmetry of the previous paragraph. But the structure of the Hamiltonians otherwise remains the same, and in particular, the shifts of the Dirac points are still given by $\vec{A}_i$ of Eq. (1).

V. ROLES OF BERRY'S PHASE IN ELECTRONIC TOPOLOGICAL TRANSITION

The characteristics of the ETT are ruled by unique interplay between the effective non-Abelian vector potential and conservation of Berry’s phase. The Berry’s phase ($\phi_B$) for each Dirac cone at $\vec{k}_{Di}$ can be calculated by using $\phi_B = \int_{\Gamma} d\vec{k} \cdot A(\vec{k})$ where $A(\vec{k}) = i \langle u_{D_i}(\vec{k}) | \partial_{\vec{R}} | u_{D_i}(\vec{k}) \rangle$, $\Gamma$ is a path enclosing each Dirac point, and $u_{D_i}(\vec{k})$ is a single-valued spinor-like eigenfunction of each Dirac Hamiltonian at $\vec{k}_{Di}$. Without sliding, we have $\phi_B = +\pi$ for the massless Dirac fermions around $\vec{k}_{D_i}$ ($i = 1, 2, 3$) and $\phi_B = -\pi$ for the ones at the center $\vec{k}_{D0}$ [Fig. 4(a)]. For a path enclosing all Dirac points at higher energy, we
can use the quadratic Hamiltonian (1) and \( \phi_D \) is \( +2\pi 5.9 \). So, the total \( \phi_D \) is always conserved to be \( 2\pi \) [Fig. 4(a)]

Now, to reveal the role of Berry's phase explicitly, let us consider exactly solvable cases without the assumption of \( |\vec{\lambda}| \ll p_D \). For sliding along \( \pm \delta_1 \) direction, i.e., \( \vec{d}_x = (0, \mp d_y) \) (\( d_y > 0 \)), the effective vector potential is given by \( \vec{A} = (\lambda_x, 0) = (\mp \beta d_y, 0) \). Here, \( \lambda_x < 0 \) (\( \lambda_x > 0 \)) when sliding along \( +\delta_1 (\pm \delta_1) \) direction. Then we have four different local vector potentials \( \vec{A_i} \) for each \( \vec{k}_{D_i} \) such that

\[
\vec{A}_0 = \frac{p_D}{2} \left( -1 + \sqrt{1 + 4\lambda_x / p_D}, 0 \right),
\quad \vec{A}_1 = \frac{p_D}{2} \left( 1 + \sqrt{1 + 4\lambda_x / p_D}, 0 \right),
\quad \vec{A}_2 = \frac{\sqrt{3} p_D}{2} \left( 0, -1 + \sqrt{1 - 4\lambda_x / 3p_D} \right),
\quad \vec{A}_3 = \frac{\sqrt{3} p_D}{2} \left( 0, 1 + \sqrt{1 - 4\lambda_x / 3p_D} \right).
\]

We note that \( \vec{A_0} + \vec{A_1} = 0 \) and \( \vec{A_2} + \vec{A_3} = 0 \). Thus, the Dirac cone at \( \vec{k}_{D0} \) and the one at \( \vec{k}_{D1} \) move in opposite direction when bilayer graphene slides along \( \pm \delta_1 \) and so do those at \( \vec{k}_{D2} \) and \( \vec{k}_{D3} \). It is also noticeable that \( \vec{k}_{D0} + \vec{A}_0 = \vec{k}_{D1} + \vec{A}_1 \) when \( \lambda_x = -p_D / 4 \) and \( \vec{k}_{D1} + \vec{A}_1 = \vec{k}_{D2} + \vec{A}_2 = \vec{k}_{D3} + \vec{A}_3 \) when \( \lambda_x = 3p_D / 4 \). Hence, when the bottom layer slides along \(-y\) direction (\( \delta_1 \) direction) by \( d_y = p_D/(4\beta) \), the two Dirac cones at \( \vec{k}_{D0} \) and \( \vec{k}_{D1} \) meet at \((-p_D/2, 0)\) while three cones at \( \vec{k}_{D1}, \vec{k}_{D2} \) and \( \vec{k}_{D3} \) meet together at \((p_D/2, 0)\) when sliding along \(+y\) direction (\( -\delta_1 \) direction) by \( d_y = 3p_D/(4\beta) \).

For the sliding along \(+\delta_1 \) direction, the effective Hamiltonian shown in Eq. (2) can be expanded around \( \vec{k} = (-p_D/2, 0) \) so that the resulting Hamiltonian can be written as

\[
\mathcal{H}_+ = \hbar v_3 \tau_x \left[ \frac{2\lambda_x}{p_D} - \left( \lambda_x + \frac{p_D}{4} \right) \right] + 2\hbar v_3 \tau_y \delta k_y \quad (5)
\]

where \( \delta \vec{k} = (\delta k_x, \delta k_y) \equiv \vec{k} - \vec{k}_+ \) and \( \lambda_x < 0 \). The new effective Hamiltonian (5) has eigenvalues given by

\[
E_+ (\delta k) = \pm \hbar v_3 \sqrt{\left[ \frac{2\lambda_x}{p_D} - \left( \lambda_x + \frac{p_D}{4} \right) \right]^2 + 4(\delta k_y)^2}.
\]

So, when \(-p_D/4 < \lambda_x < 0 \) or \( 0 < d_y < p_D/(4\beta) \), there are still two Dirac cones at \( \vec{k}_{D0} + \vec{A}_0 \) and \( \vec{k}_{D1} + \vec{A}_1 \). When \( \lambda_x \) reaches to a critical value of \(-p_D/4\), the Hamiltonian is given by \( \hbar v_3 \tau_x (\delta k_x)^2 / p_D + 2\hbar v_3 \tau_y \delta k_y \) so that the dispersion along \( k_x \) direction is massive while one along \( k_y \) direction is still massless. Two other cones at \( \vec{k}_{D2} + \vec{A}_2 \) and \( \vec{k}_{D3} + \vec{A}_3 \) move away from each other in \( \pm k_y \) direction maintaining their anisotropic Dirac cone shapes. Therefore, it can be seen that the cones at \( \vec{k}_{D0} \) and \( \vec{k}_{D1} \) merge together when \( \vec{A} = (-p_D/4, 0) \) [Fig. 4(c)]. The
corresponding sliding distance of $d_y$ is about 0.3% of $a_c$ ($d_y = p_D/(4\beta) \sim 0.004\AA$). The low energy bands already change their topology from the original structure under extremely small sliding. For further sliding, $\lambda_x < -p_D/4$ ($d_y > p_D/(4\beta)$), the merged cone eventually disappears and the spectrum of Eq. (6) develops an energy gap at $\tilde{k}_c$ as shown in Fig. 4(d). The gap is linear with sliding distance as given by $2h v_3|\lambda_x + p_D/4| \approx 2h v_3d_y \sim 0.9 \times |d_y/a_c| \text{ eV}$. The opening of energy gap signals a pair annihilation of two massless Dirac electrons with the opposite ‘topological charges’ of ±1 since the two Dirac cones at $\tilde{k}_{D0}$ and $\tilde{k}_{D1}$ have the Berry’s phase of $\pm \pi$ respectively. This also confirms the Berry’s phase conservation since the remaining two anisotropic Dirac cones at $\tilde{k}_{D2}$ and $\tilde{k}_{D3}$ give the total $\phi_B$ of $2\pi$.

Next, for the sliding along $-\tilde{\delta}_1$ direction, the effective Hamiltonian can be obtained by expanding Eq. (2) around $\tilde{k}_- = (p_D/2, 0)$:

$$\mathcal{H}_- \simeq \hbar v_3 \tau_x \left[2\delta k_x + \frac{(\delta k_x)^2 - (\delta k_y)^2}{p_D} + \left(\frac{3p_D}{4} - \lambda_x\right)\right] + 2h v_3 \tau_y \left(\frac{\delta k_x}{p_D}\right),$$

(7)

where $\delta k = (\delta k_x, \delta k_y) \equiv \tilde{k} - \tilde{k}_-$ and $\lambda_x > 0$. When $0 < \lambda_x < 3p_D/4$, there are three Dirac cones at $\tilde{k}_{D1} + \tilde{A}_1$ (i = 0, 2, 3). However, when $\lambda_x = 3p_D/4$, the three Dirac cones merge at $\tilde{k}_-$ and this Hamiltonian gives an anomalous dispersion relation written by $E_-(\delta k) = \pm \hbar v_3 f^2(\delta k) + g^2(\delta k)$ where $f(\delta k) = 2\delta k_x + (\delta k_x)^2/p_D - (\delta k_y)^2/p_D$ and $g(\delta k) = 2(\delta k_x)(\delta k_y)/p_D$. This gives sickle-shaped constant energy contours which are consistent with our $ab initio$ calculation results shown in Figs. 3(e) and (g). When $\lambda_x > 3p_D/4$, the effective Hamiltonian (7) does not develop any energy gap at all. Instead, when $\lambda_x \gg 3p_D/4$, the effective Hamiltonian has a Dirac point at $\tilde{k}_- = (-p_D/2 + \sqrt{\lambda_x p_D}, 0)$ and is given by

$$\mathcal{H}'_- \simeq 2\hbar v_3 \left(\frac{\lambda_x}{p_D}\right) \tau_x^* \delta k_x + 2h v_3 \left(\frac{\lambda_x}{p_D} - 1\right) \tau_y^* \delta k_y,$$

(8)

where $\delta k = (\delta k_x, \delta k_y) \equiv \tilde{k} - \tilde{k}_-$. So, as sliding distance increases along $-\tilde{\delta}_1$, the anomalous Hamiltonian (7) gradually transforms to the anisotropic Dirac Hamiltonian (8). This is quite contrary to the gapped spectrum (6) generated by sliding motion along $\tilde{\delta}_1$ direction ($\mathcal{H}_+$ in Eq. (5)). The other cone at $\tilde{k}_{D1} + \tilde{A}_1$ moves in $-k_x$ direction maintaining its anisotropic dispersion relation. As $\lambda_x \gg 3p_D/4$, the Dirac cone at $\tilde{k}_{D1} + \tilde{A}_1$ has an asymptotic shape as following,

$$\mathcal{H}''_n \simeq -2\hbar v_3 \left(\frac{\lambda_x}{p_D}\right) \tau_x^* \delta k_x - 2h v_3 \left(\frac{\lambda_x}{p_D} + 1\right) \tau_y^* \delta k_y,$$

(9)

where $\tilde{k} = (\delta k_x, \delta k_y) \equiv \tilde{k} - \tilde{k}_{D1} - \tilde{A}_1$. Therefore, in contrast to the first case, no energy gap develops even when the sliding distance is increased further. Instead, the anomalous dispersion transforms to an anisotropic Dirac cone [Fig. 4(g)]. This phenomenon can be interpreted as a merging of two massless fermions of topological charge +1 with one of topological charge −1. As a result, a new fermion of topological charge $+1$ is generated. We note that the total $\phi_B$ of $2\pi$ is conserved since the new particle has $\phi_B$ of $\pi$. Hence, the topocharge births of fermionic particles in BLG are strictly governed by Berry’s phase conservation rule.

VI. EFFECT OF SMALLEST INTERLAYER HOPPINGS

When sliding occurs, the smallest interlayer interaction $\gamma_4$ shown in Fig. 1(c) becomes anisotropic and depends on the pair distances between relevant carbon atoms in the top and bottom layer. This effect adds an additional Hamiltonian to Eq. (2),

$$\mathcal{H}'_n \simeq \frac{2\hbar^2 v_0 v_4}{\gamma_1} \sum_{k} \left(\vec{k} \cdot \vec{\lambda}\right) \tau_0 + \frac{\hbar^2 v_2^2}{\gamma_1} \left[\tau^* \cdot (\vec{k} + \vec{\lambda})\right] \tau_x \left[\tau^* \cdot (\vec{k} + \vec{\lambda})\right],$$

(10)

where $v_4 = \frac{3\pi a_c}{2}\gamma_1$ (See Appendix for derivation of Eq. (10)). Since the second term in Eq. (10) is twenty times smaller than the first term, we will neglect the second term hereafter. When sliding along $-\tilde{\delta}_1$, the difference between Dirac energies at $\tilde{k}_{D1}$ and $\tilde{k}_{D0}$ is given by $\frac{2\pi 4}{v_0} \sqrt{1 + \frac{3\lambda_x}{p_D}}$. Without sliding ($\lambda_x = 0$), the difference becomes $\Delta \varepsilon_{\text{eh}} = \frac{2\pi 4}{v_0}$, which indicates the hole and electron doped Dirac cone at $\tilde{k}_{D1}$ and $\tilde{k}_{D0}$ respectively. This explains the hole and electron doped cones shown in our $ab initio$ calculation results [Fig. 3(b)]. With sliding along $\tilde{\delta}_1$, the difference disappears when $\lambda_x < -p_D/4$ as shown in Figs. 3(c) and 3(d) so that all Dirac cones are charge-neutral. Contrary to this, when sliding along $-\tilde{\delta}_1$, the difference changes its sign when $\lambda_x > p_D$ and decreases significantly as sliding distance increases. So, the hole-doped Dirac cone at $\tilde{k}_{D1}$ changes to be electron-doped and the new Dirac cone to be hole-doped with increasing amount of doping as increasing sliding distance as shown in our first-principles calculations [Figs. 3(e)-(h)]. We note that variations in $\gamma_4$ do not affect any topological changes discussed so far.

VII. DISCUSSION

The direct signatures of the ETT can be readily measured using various experiment methods. We showed that the tiny sliding lifts the degeneracy at $E_F$ as the
principles calculations indeed show drastic variations in linearly depends on energy,

\[ \kappa(x) \]

onto \( \kappa \) (d) \( x \)

When BLG slides along \( \pm \kappa \) (g), respectively, where \( \kappa \) (d) is an area of closed orbit of electron and \( \gamma = 1/2 - \phi B/2 \). We can immediately confirm that the Landau level (LL) spectrum under a small magnetic field is given by \( E_n \sim (Bn)^{1/2} \) in the case of sliding BLG along \( \kappa(x) = 0.02 \delta_1 \). When BLG slides by either \( -0.02 \delta_1 \) or \( 0.012(\kappa_3 - \delta_1) \), the anomalous Dirac cone shape results in \( D(E) \sim \sqrt{E} \) being similar to the previous study on the density of states of semi-Dirac cone (massive in one direction and massless in the other). By using the rule above and \( D(E) \sim \sqrt{E} \), the LL spectrum is given by \( E_n \sim (Bn)^{2/3} \). It is noticeable that, irrespective of sliding direction, the zeroth LL exists at zero energy since the topological charge conservation (Berry’s phase conservation) enforce the existence of at least one massless modes in the system.

Third, an ideal minimal conductivity of \( 24e^2/(\pi^2\hbar) \) at the charge neutral point \( (B\pi^2/2e^2) \) will decrease quickly when sliding occurs \( (e \) is the electron charge). The conductivity of anisotropic massless Dirac fermions with a dispersion, \( v_x \tau_x k_x + v_y \tau_y k_y \), is given by \( \sigma = g^2 v^2/2e^2 \). Here \( g \) is a degeneracy factor \( (g = 4 \) if considering valley and spin degeneracies) and \( e \) is an electron charge. So, by using Eqs (8) and (9), the conductivity in wide BLG sliding along \( \delta_1 \) \( (a_g \gg p_D) \) can be calculated easily, \( \sigma = g^2 v^2(1 - p_D/\lambda_d) \gamma^2 \sim g^2(1 + p_D/\lambda_d) \). The conductivity approaches \( 8e^2/(\pi^2\hbar) \) as sliding distance increases.

In summary, we show that the topology of energy bands of BLG changes significantly if sliding of extremely small distance occurs in any direction. The effective non-Abelian background gauge potential can be generated by sliding motion and is shown to play an important role in dictating the characteristics of sliding induced ETT. Hence, the ETT driven by non-Abelian gauge fields that are thought to be possible in cold atomic gases or similar effects in high energy physics can be realizable in sliding BLG.

Note added in proof After submission, we became aware of related works on similar systems from other groups.

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Appendix: Derivation of Eqs. (2) and (10)

A single particle Hamiltonian of BLG in Bernal stacking, \( H = H_0 + H_1 + H_2 \), can be written as

\[
H_0 = -\gamma_0 \sum_{\vec{r}, j, \alpha} a_\alpha^\dagger(\vec{r}) b_\alpha(\vec{r} + \vec{\delta}_j) + (\text{h.c.}), \quad (A.1)
\]

\[
H_1 = -\gamma_1 \sum_{\vec{r}} a_1^\dagger(\vec{r}) b_2(\vec{r}) - \frac{\gamma_3}{2} \sum_{\vec{r}, \vec{j}} a_2^\dagger(\vec{r} + \vec{\delta}_j) b_1(\vec{r}) + (\text{h.c.}), \quad (A.2)
\]

\[
H_2 = -\gamma_4 \sum_{\vec{r}, \vec{j}} a_1^\dagger(\vec{r} + \vec{\delta}_j) a_2(\vec{r}) - 2 \gamma_4 \sum_{\vec{r}, \vec{j}} b_1^\dagger(\vec{r} + \vec{\delta}_j) b_2(\vec{r}) + (\text{h.c.}), \quad (A.3)
\]

where \( H_0 \) is a Hamiltonian for intra-layer interactions in each SLG and \( H_1 \) and \( H_2 \) are for inter-layer interactions between two SLG. Here \( a_\alpha^\dagger(\vec{r}) \) and \( b_\alpha(\vec{r}) \) are the creation (annihilation) operator of \( \pi \)-electron located at \( \vec{r} \) and \( \alpha = (1, 2) \) respectively, where \( \vec{r} = m \vec{a}_1 + n \vec{a}_2 \) and \( \vec{\delta}_j = (\vec{\delta}_3 - \vec{\delta}_1) \) are unit vectors of hexagonal lattice of SLG. \( \gamma_0 \) is the intra-layer nn hopping parameter, and \( \gamma_1 \) and \( \gamma_3 \) are for the nn and next nn (nnn) inter-layer hopping parameters, respectively.

Using Fourier transformations of \( a_\alpha(\vec{r}) = \frac{1}{\sqrt{N}} \sum_\vec{p} e^{-i\vec{p} \cdot \vec{r}} a_\alpha(\vec{p}) \) and \( b_\alpha(\vec{r}) = \frac{1}{\sqrt{N}} \sum_\vec{p} e^{-i\vec{p} \cdot \vec{r}} b_\alpha(\vec{p}) \) (\( N \) is a total number of unitcells), the total Hamiltonian \( (H) \) in Eqs. (A.1)-(A.3) can be written in a matrix form such as \( H = \sum_\vec{p} \Psi_\vec{p}^\dagger H_{\vec{p}} \Psi_\vec{p} \) for a field of \( \Psi_\vec{p} = (h_{1\vec{p}}, a_{2\vec{p}}, a_{1\vec{p}}, b_{2\vec{p}})^T \) where

\[
H_{\vec{p}} = \begin{pmatrix}
\xi_1(p) & \xi_0(p) & \xi_4(p) & \xi_5(p) \\
\xi_0(p) & 0 & \xi_2(p) & \xi_3(p) \\
\xi_4(p) & \xi_2(p) & 0 & -\gamma_1 \\
\xi_5(p) & \xi_3(p) & \xi_0(p) & -\gamma_1 
\end{pmatrix}, \quad (A.4)
\]

and \( \xi_\alpha(p) = -\gamma_0 \sum_j e^{i\vec{p} \cdot \vec{\delta}_j} (\alpha = 0, 3, 4, j = 1, 2, 3) \). When we expand Eq. (A.4) around \( K \)-point by using \( \vec{p} = \vec{k} + \vec{K} \) \( (|\vec{k}| \ll |\vec{K}|) \) and \( \vec{K} = (\frac{\sqrt{3}}{2} a_1, 0, 0) \),

\[
\xi_\alpha(\vec{k} + \vec{K}) \approx -\gamma_0 \sum_j e^{i\vec{K} \cdot \vec{\delta}_j} - i\gamma_0 \sum_j \vec{k} \cdot \vec{\delta}_j e^{i\vec{K} \cdot \vec{\delta}_j} = v_\alpha(k_x + ik_y), \quad (A.5)
\]

where \( v_\alpha = \frac{\sqrt{3}}{2\hbar} \gamma_0 c_\alpha \) (\( \alpha = 0, 3, 4 \)), \( \hbar \) is the Planck constant, and \( \hbar \vec{k} = \hbar(k_x, k_y) \) is the crystal momentum from \( K \)-point. The total Hamiltonian near \( K \)-point for a field \( \Psi_\vec{k} = (b_{1\vec{k}}, a_{2\vec{k}}, a_{1\vec{k}}, b_{2\vec{k}})^T \) can be written as

\[
H_\vec{k} = \hbar \begin{pmatrix}
v_3 k_x & v_0 k_y & v_2 k_y & v_4 k_y \\
v_3 k_x & 0 & v_0 k_y & -v_2 k_y \\
v_0 k_y & v_4 k_y & 0 & -\gamma_1 \\
v_2 k_y & v_4 k_y & -\gamma_1 & 0 
\end{pmatrix}, \quad (A.6)
\]

where \( k_\pm = k_x \pm ik_y \). The effective Hamiltonian \( (H_{\text{eff}} + H'_{\text{eff}}) \) on the low energy electronic structures for a field \( \Psi_\vec{k} = (b_{1\vec{k}}, a_{2\vec{k}})^T \), are described by

\[
H_{\text{eff}} \approx \hbar v_3 \begin{pmatrix} 0 & k_x \\ k_x & 0 \end{pmatrix} + \frac{\hbar^2 v_2^2}{\gamma_1} \begin{pmatrix} 0 & k_y^2 \\ k_y & 0 \end{pmatrix}, \quad (A.7)
\]

\[
H'_{\text{eff}} \approx \frac{2\hbar v_0 v_4}{\gamma_1} \begin{pmatrix} k_x & 0 \\ k_x & k_y \end{pmatrix} + \frac{\hbar^2 v_3^2}{\gamma_1} \begin{pmatrix} k_y^2 & 0 \\ 0 & k_y^2 \end{pmatrix}. \quad (A.8)
\]

Here we decompose the effective Hamiltonian into \( H_{\text{eff}} \) and \( H'_{\text{eff}} \) where the latter is quite small compared to the former. By using Pauli spin matrices, \( \tau_0 = (1, 0, 0) \) and \( \tau_x = (0, 1, 0) \), and \( \tau_y = (0, 0, 1) \), the above Eqs. (A.7) and (A.8) can be written in compact forms,

\[
H_{\text{eff}} \approx \hbar v_3 \vec{\tau} \cdot \vec{k} + \frac{\hbar^2 v_2^2}{\gamma_1} (\vec{\tau} \times \vec{k}) \tau_z (\vec{\tau} \times \vec{k}), \quad (A.9)
\]

\[
H'_{\text{eff}} \approx \frac{2\hbar v_0 v_4}{\gamma_1} |\vec{k}|^2 \tau_0 \tau_x (\vec{\tau} \times \vec{k}), \quad (A.10)
\]

where \( \vec{\tau} = (\tau_x, \tau_y) \) and \( \vec{\tau}^* \) is its complex conjugate. Hereafter, we will neglect the smallest hopping parameter \( \gamma_4 \) (Eqs. (A.8) and (A.10)) and discuss its role later.

The effective Hamiltonian in Eq. (A.9) gives energy eigenvalues

\[
E(\vec{k}) = \pm \hbar v_3 |k| + \frac{\hbar^2 v_2^2}{\gamma_1} |k|^2, \quad (A.11)
\]

where \( \phi_\ell = \tan^{-1}(k_y/k_x) \) and \( p_D = \gamma_1 v_3/(\hbar v_0^2) = 2/(3a_\ell)(\gamma_1 \gamma_3/\gamma_0^2) \).

When the layer 2 (bottom layer) slides against the layer 1 (top) along \( a_\ell' = (a_x, a_y) \) \( (|a_\ell'| \ll a_\ell) \)[Figs. 1(a) and (b)], the constant nn inter-layer interaction \( (\gamma_3) \) now depends on the carbon pair distance in layer 1 and 2 \( (|d_\ell'|) \) and nn inter-layer interaction \( (\gamma_3) \) decreases to \( \gamma_3' \). Since we focus on an extremely small sliding distance, we assume variation of the nn inter-layer interaction such as \( \gamma_3 \rightarrow \gamma_3(\delta) \approx \gamma_3 e^{-\delta a_\ell} \), \( \delta \approx \gamma_3 (1 - \beta \delta_1 \cdot d_\ell) \) where \( i = 1, 2, 3 \) and \( \beta \) is a positive real constant. When we expand Eq. (A.4) around \( K \)-point including sliding effect, interlayer interactions remain the same as before. However, unlike the expansion procedure without sliding shown in Eq. (A.5), the interlayer interaction with sliding can be
expanded up to a leading order of $\vec{k}$ and $\vec{d}$ as

$$
\xi_3(\vec{k} + \vec{K}) \simeq -\sum_j \gamma_3(\delta_j) e^{i(\vec{k} + \vec{K}) \cdot \delta_j}
\simeq -\sum_j \gamma_3(1 - \beta \delta_i \cdot \vec{d}_j)(1 + ik \cdot \vec{d}_j)e^{i\vec{K} \cdot \delta_j}
\simeq \hbar v_3(k_x + ik_y) + \hbar v_3\beta(id_x - d_y).
\quad (A.12)
$$

Hence, the sliding vector $d_y$ plays a role of shifting the unn intra-layer Hamiltonian in momentum space like a constant vector potential. With $\gamma_4$ neglected, the total Hamiltonian near $K$-point in Eq. (A.9) now transforms to

$$
\mathcal{H}_K = \hbar \left( \begin{array}{cccc}
0 & v_3(k_x - \lambda_-) & v_0k_+ & 0 \\
v_0k_- & 0 & 0 & -\gamma_1 \\
0 & v_0k_+ & 0 & -\gamma_1 \\
\end{array} \right)
\quad (A.13)
$$

where $\lambda_\pm = \beta(d_y \pm i d_x)$. Here we neglect an overall phase shift of $e^{i\pi\delta_2\cdot\vec{k}}$ because of $|\delta_1| \ll a_c$. The effective low energy Hamiltonian of Eq. (A.9) also changes to

$$
\mathcal{H}_{\text{eff}} \simeq \hbar v_3\vec{\tau} \cdot (\vec{k} - \vec{\lambda}) + \frac{\hbar^2 v_0^2}{\gamma_1}(\vec{\tau}^* \cdot \vec{k})\tau_x(\vec{\tau}^* \cdot \vec{\lambda}).
\quad (A.14)
$$

where $\vec{\lambda} \equiv (\lambda_x, \lambda_y) = \beta(d_y, -d_x) = \beta(\vec{d}_x \times k_z) (k_z = k_x \times k_y)$ and $(\vec{k}_x, \vec{k}_y) = \vec{k}/|\vec{k}|$.

Now, let us consider the smallest interlayer interaction $\gamma_4$ with sliding. When sliding occurs, $\gamma_4$ shown in Fig. 1(e) becomes anisotropic and depends on the pair distances between relevant carbon atoms in the top and bottom layer. We find that $\gamma_4 \rightarrow \gamma_4(\delta) \simeq \gamma_4 e^{i\beta \delta \cdot \vec{d}} \simeq \gamma_4(1 + \beta \delta_i \cdot \vec{d}_j)$ where $i = 1, 2, 3$. Here we assume the same coefficient $\beta$ of $\gamma_3(\delta)$ for calculation convenience and note that it does not change the main conclusions of the paper. Like Eq. (A.12) for $\gamma_3$, we can expand $\xi_4$ as

$$
\xi_4(\vec{k} + \vec{K}) \simeq -\sum_j \gamma_4(\delta_j) e^{i(\vec{k} + \vec{K}) \cdot \delta_j}
\simeq -\sum_j \gamma_4(1 + \beta \delta_i \cdot \vec{d}_j)(1 + ik \cdot \vec{d}_j)e^{i\vec{K} \cdot \delta_j}
\simeq \hbar v_4(k_x + ik_y) - \hbar v_4\beta(id_x - d_y)
= \hbar v_4 k_x + \hbar v_4\lambda_+.
\quad (A.15)
$$

With $\gamma_4$ included, now the total Hamiltonian near $K$-point in Eq. (A.13) has an additional term,

$$
\mathcal{H}_K = \hbar v_4 \left( \begin{array}{cccc}
0 & 0 & 0 & k_+ + \lambda_+ \\
0 & 0 & k_- + \lambda_- & 0 \\
0 & k_- + \lambda_- & 0 & 0 \\
\end{array} \right)
\quad (A.16)
$$

Then, Eq. (A.10) changes to

$$
\mathcal{H}_{\text{eff}}' \simeq \frac{2\hbar^2 v_0 v_4}{\gamma_1} \vec{k} \cdot (\vec{k} + \vec{\lambda})\tau_0
+ \frac{\hbar^2 v_0^2}{\gamma_1}(\vec{k}^* \cdot \vec{\lambda})\tau_x(\vec{k}^* \cdot (\vec{k} + \vec{\lambda})).
\quad (A.17)
$$
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