Orbital mixing in few-layer graphene and non-Abelian Berry phase

K. Shizuya
Yukawa Institute for Theoretical Physics
Kyoto University, Kyoto 606-8502, Japan

In a magnetic field few-layer graphene supports, at the lowest Landau level, a multiplet of zero-mode levels nearly degenerate in orbitals as well as in spins and valleys. Those pseudo-zero-mode (PZM) levels are generally sensitive to interactions and external perturbations, and have a crossing among themselves or with other higher Landau levels when an external field is swept over a certain range. A close study is made of how such PZM levels evolve when they are gradually brought from empty to filled levels under many-body interactions. It is pointed out that the level spectra generally avoid a crossing via orbital level mixing and that orbital mixing is governed by a non-Abelian Berry phase that derives from an approximate degeneracy and interactions. A look is also taken into evolution/crossing of many-body ground states with increasing external bias in bilayer graphene.

I. INTRODUCTION

Graphene hosts massless Dirac electrons as charge carriers that display fascinating electronic properties. Recently considerable attention centers on graphene bilayers and few-layers, where the added layer degrees of freedom open a new realm of physics and applications with, e.g., a tunable band gap in bilayer graphene. Trilayers acquire a three-fold degeneracy in orbitals. This orbital degeneracy has a topological origin in the index of (the leading part of) the one-body Dirac Hamiltonian. In the presence of spin and band anisotropies and many-body interactions, these zero-mode levels evolve into pseudo-zero-mode (PZM) levels, or into a variety of broken-symmetry multiplets of different orbitals and explored experimentally. It was noted, in particular, that the orbital degeneracy is also lifted by Coulomb interactions alone, with the zero-energy modes orbitally Lamb shifted due to quantum fluctuations of the filled valence band. The orbital degeneracy and its lifting by the orbital Lamb shift are new features specific to the LLL in few-layer graphene.

Those PZM levels are generally sensitive to external perturbations and have a chance of crossing among themselves or with other higher Landau levels when an external field is swept over a certain range. Many-body interactions significantly affect such level-crossing phenomena. To see this, let us suppose that two empty levels, that differ only in orbitals \( n \) and \( m \) \((n > m \geq 0)\), have a crossing when an external field \( u \) is varied across a critical value \( u_{cT} \), as depicted in Fig. 1(a), and ask what happens when one fills them with electrons. If there is no electron-electron interaction, the level spectra remain unchanged and the filled levels continue to have a crossing at \( u_{cT} \).

In the presence of interaction, the level spectra are lowered by the amount of exchange energies, and the filled levels lose a crossing at \( u \sim u_{cT} \), or the crossing point gets shifted, \( u_{cT} \rightarrow u'_{cT} \), as illustrated in the figure. (Note that the exchange energy \( \epsilon_n^x < 0 \) generally decreases with increasing orbital index \( n \); \( |\epsilon_n^x| < |\epsilon_m^x| \) for \( n > m \geq 0 \).) The two levels, as they are gradually filled, thus appear to cross for \( u \in (u'_{cT}, u_{cT}) \) while no crossing is expected for \( u > u_{cT} \).

Experimentally a similar many-body phenomenon of spin exchange energy origin has been known: In a GaAs/AlGaAs quantum well with doubly occupied subbands, crossings of two Landau levels of different subbands lead to ring-like structures in the phase diagram that suggest transitions due to spin exchange energy.

The purpose of the present paper is to examine how those nearly degenerate PZM levels behave when they are gradually brought from empty to filled levels under many-body interactions. It is pointed out that the level spectra generally avoid a crossing via orbital level mixing and that orbital mixing is governed by a non-Abelian Berry phase that derives from an approximate degeneracy and interactions. This non-Abelian phase clar-

FIG. 1. Orbital level crossing. (a) Two empty levels (dotted lines) of different orbitals \( n \) and \( m \) undergo a crossing with increasing external bias \( u \). When they are filled up (solid lines), the crossing point gets shifted \( (u'_{cT} \rightarrow u'_{cT} \) due to orbit-dependent Coulombic exchange energies, causing a level inversion for \( u \in (u'_{cT}, u_{cT}) \). (b) Renormalized PZM level spectra \( (\tilde{\epsilon}_0, \tilde{\epsilon}_1) \) in bilayer graphene, plotted as a function of external bias \( u \). A level inversion takes place for \( 0 \leq u < u_{cT} \) in valley \( K \) and for \( -u_{cT} < u \leq 0 \) in valley \( K' \).
ifies the algebraic features underlying the phenomena of Landau-level crossing and mixing. We also examine, as a typical case of crossing of many-body states, how the neutral ($\nu = 0$) ground state in bilayer graphene evolves with increasing interlayer bias $u$.

In Sec. II we briefly review some basic features of the PZM levels in bilayer graphene. In Secs. III and IV, we examine the level-mixing phenomenon and its algebraic character in the light of a non-Abelian Berry phase. In Sec. V we look into trilayer graphene and show that the Berry phase encodes and distinguishes possible patterns of orbital mixing in different types of trilayers. In Sec. VI we examine evolution of the $\nu = 0$ ground state in bilayer graphene with bias $u$. Section VII is devoted to a summary and discussion.

II. THE LOWEST LANDAU LEVEL IN BILAYER GRAPHENE

In a magnetic field $B_z = B$ one-body states $|n, y_a; a, \alpha\rangle$ of a Dirac electron in graphene are labelled by integers $n = 0, \pm 1, \pm 2, \cdots$ and momentum $p_x$ (or the center-coordinate $y_0 = \ell^2 p_x$ with the magnetic length $\ell \equiv 1/(\sqrt{eB})$, as well as valleys $a \in (K, K')$ and spins $\alpha \in (\uparrow, \downarrow)$. The associated one-body Hamiltonian is generally written as

$$H^{1b} = \int d y_0 \sum_{n, a, \alpha} \psi^{n,a\dagger}_\alpha(y_0) \epsilon_{\alpha}^{n,a} \psi^{n,a}_\alpha(y_0),$$

where $\psi^{n,a}_\alpha(y_0)$ denotes the electron field with the spectrum $\epsilon_{\alpha}^{n,a}$; $\psi^{n,a}_\alpha(y_0) \equiv \int d^2x \langle n, y_a; a, \alpha|x|\Psi_x\rangle$ in terms of the field $\Psi_x$ in the coordinate space. The charge density $\rho_{-p} = \int d^2x e^{ip\cdot x} \Psi_x^{\dagger}\Psi_x$ is thereby written as

$$\rho_{-p} = \gamma_p \sum_{m, a, n, -\infty} \sum_{a, \alpha} \mathfrak{g}_{m; n; a, \alpha} R_{a, \alpha; -p, m},$$

$$R_{a, \alpha; -p, m} \equiv \int d y_0 \psi^{m,a\dagger}_\alpha(y_0) e^{ip\cdot r} \psi^{n,b}_\alpha(y_0),$$

with $\gamma_p \equiv e^{-\gamma_p^2/4}$; $r = (it^2 \partial/\partial y_0, y_0)$ stands for the center coordinate with uncertainty $[r_x, r_y] = it^2$. The projected charges $\mathfrak{g}_{m; n; a, \alpha}$ obey the Weyl algebra \[\mathfrak{g}\]. The coefficient functions $\mathfrak{g}_{m; n; a, \alpha}$ have the structure

$$\mathfrak{g}_{m; n; a, \alpha} \propto p^{m-n} \times \text{(polynomials of } \ell^2 p^2) \text{ for } |m| \geq |n|,$$

$$\text{and } \mathfrak{g}_{m; n; a, \alpha} = (\mathfrak{g}_{m; n; a, \alpha})^\dagger,$$

and $p = p_x + i p_y$.

For bilayer graphene the one-body spectra $\{\epsilon_{\alpha}^{n,a}\}$ take an electron-hole ($e-h$) symmetric pattern when only the leading intralayer and interlayer couplings $\gamma_0 = \gamma_{AB} \sim 3$ eV (related to the Fermi velocity $v \sim 10^6$ m/s in monolayer graphene) and $\gamma_1 \equiv \gamma_{A'B'} \sim 0.4$ eV are kept. For simplicity, nonleading couplings ($\Delta, \gamma_4, \cdots$) that lead to weak $e-h$ breaking $[31, 32]$ are suppressed in what follows; spin splitting is to be restored in Sec. VI.

The Coulomb interaction is written as

$$V^C = \frac{1}{2} \sum_{\mathbf{p}} \nu_{\mathbf{p}} \rho_{-\mathbf{p}} \rho_{\mathbf{p}}; \text{ with potential } \nu_{\mathbf{p}} = 2re_{\alpha}^{n,a}/(e_{\alpha}^{n,a} |\mathbf{p}|),$$

$$\text{and the substrate dielectric constant } \varepsilon_s;$$

$$\sum_{\mathbf{p}} = \int d^2p/(2\pi)^2 \text{ and } : \text{ denotes normal ordering. For simplicity, we ignore a tiny interlayer separation } d \to 0.$$ It is advantageous to cast $V^C$ in the form of manifest exchange interaction,

$$V^C = -\frac{1}{2} \sum_k \nu_{k}^{j;j;mn;ab} R_{a, \alpha; -k, b}^\dagger R_{a, \alpha; k, b}^\dagger,$$

with the dual potential

$$\nu_{k}^{j;j;mn;ab} = \frac{1}{\rho} \sum_{\mathbf{p}} \nu_{\mathbf{p}} \rho_{\mathbf{p}}^{a, \alpha} g_{k;\mathbf{p}}^{a, \alpha} g_{-\mathbf{p}}^{b, \beta} e^{i |\mathbf{p}| \times |\mathbf{k}|},$$

where $\rho = 1/(2\pi \ell^2)$ and $\mathbf{p} \times \mathbf{k} = p_x k_y - p_y k_x$. (For clarity, summation over repeated labels will be suppressed from now on.) This direct-exchange duality of the Coulomb interaction is made manifest on the operator level \[33\] for planar electrons in a magnetic field, where interaction becomes short-ranged with a cutoff $\sim \ell$.

In bilayer graphene an octet of PZM levels, nearly degenerate in spins, valleys and orbitals $n = \{0, 1\}$, forms the LLL isolated from other Landau levels. A key feature is a band gap which is tunable \[2, 3\] by an applied interlayer bias $u$. Actually, bias $u$ splits valleys $(K, K')$ and the bare spectra have the following valley structure,

$$\epsilon_{K}^{\pm} = -\epsilon_{K}^{\pm} \equiv \epsilon_{K}^{\pm} \equiv \epsilon_{K}^{\pm} \equiv \epsilon_{K}^{\pm},$$

$$\epsilon_{-u} \equiv \epsilon_{K}^{-u} \equiv \epsilon_{K}^{-u} \equiv \epsilon_{K}^{-u},$$

where $O|-u$ signifies setting $u \to -u$ in $O$. Here each $n = \pm 2, \pm 3, \ldots$ refers to a pair of electron and hole levels. In contrast, the PZM levels $n = \{0, 1\}$ stand alone (per spin and valley) and are $e-h$ self-conjugate, with $\pm n \to n$ in Eq. \[6\]. Their spectra read \[17\]

$$\epsilon_{K}^{\pm} = -\epsilon_{K}^{\pm} \equiv \epsilon_{K}^{\pm} \equiv \epsilon_{K}^{\pm},$$

$$\epsilon_{z} = 1 - 2/(g^2 + 1) + O(u^2/g^2 \omega_c^2) < 1,$$

where $g \equiv \gamma_1/\omega_c$ and

$$\omega_c \equiv \sqrt{v / \ell} \approx 36.3 \times v [10^6 \text{ m/s}] \sqrt{B[T]} \text{ meV}$$

is the characteristic cyclotron energy of graphene. Note that $\epsilon_1$ has a slightly smaller gradient $(z_1 < 1)$ in bias $u$ than $\epsilon_0$. As for band parameters \[34\], we adopt $v = 0.845 \times 10^6$ m/s and $\gamma_1 = 361$ meV so that $\omega_c \approx 137$ meV, $g \approx 2.63$ and $z_1 \approx 0.75$ at $B = 20$ T.

Interlayer bias $u$ shifts the PZM levels $n = \{0, 1\}$ oppositely ($\pm u/2$) in the two valleys. We take, without loss of generality, $u \geq 0$ for valley $K$; $u < 0$ then refers to $K'$. The valley gap $\sim u$ increases with bias $u$ while $(\epsilon_1, \epsilon_2)$ remain nearly degenerate in each valley.

For the PZM levels, form factors $g_{m; n; a, \alpha}$ take particularly simple form

$$g_{0}^{m; n; a, \alpha} = 1, \quad g_{1}^{m; n; a, \alpha} = 1 - c_{\alpha}^{m; n; a, \alpha} p^2,$$

$$g_{0}^{m; n; a, \alpha} = c_{\alpha}^{m; n; a, \alpha} p/\sqrt{2}, \quad g_{0}^{m; n; a, \alpha} = -c_{\alpha}^{m; n; a, \alpha} p^1/\sqrt{2},$$

where $\alpha \equiv \gamma_1/\omega_c$ and
with $c_1|K' = c_1|K_{-u}$; in $e$-$h$ symmetric setting,

$$ c_1 \approx 1/ \sqrt{1 + (1/g^2)^2} \sim 0.93 $$

(11)

scarcely depends on bias $u$ and valleys.

Electrons in each Landau level are subject to Coulombic quantum fluctuations of the filled valence band. The exchange interaction gives rise to $O(V^C)$ self-energy corrections to level spectra $\epsilon_n^{m,\alpha}$ of the form

$$ \delta \epsilon_{m,\alpha} = - \sum_p v_p^2 \frac{\gamma_p}{v_p} \sum_m v_{m,\alpha}^2 \rho^{m,m}_{n} |^2, $$

(12)

where $0 \leq v_{m,\alpha}^2 \leq 1$ stands for the filling fraction of the $(m, a, \alpha)$ level. The direct interaction leads to corrections $\propto v_{p \rightarrow 0}$, which, as usual, are removed when the neutralizing background is assumed. The exchange energy acts separately for each (valley, spin) channel. We thus suppress those labels below and mainly refer to valley $K$. We use $0 \leq N_f \leq 2$ to specify the filling fraction of the PZM sector $n = \{0, 1\}$ (per spin and valley), with $N_f = 0$ for the empty sector and $N_f = 2$ for the filled one.

Let us now consider an empty PZM sector with levels below it all filled, i.e., $v_{n,\alpha}^2 = 1$ for $n \leq -2$. Infinitely many filled levels in the valence band make self-energies $\delta \epsilon_{m,\alpha}$ ultraviolet divergent, and one has to go through renormalization of band parameters $v$ and $\gamma_1$. See Ref. [13] for details of the renormalization procedure. The empty PZM levels in valley $K$, e.g., acquire the following renormalized spectra

$$ \hat{\epsilon}_0|_{N_f=0} = - \frac{1}{\delta_b} u + \Omega_0 + \frac{1}{2}(1 + \frac{1}{4} C^2) \tilde{V}_c, $$

$$ \hat{\epsilon}_1|_{N_f=0} = - \frac{1}{2} \frac{1}{\delta_b} u + \Omega_1 + \frac{1}{2}(1 + \frac{1}{4} C^2 - \frac{1}{4} C) \tilde{V}_c, $$

(13)

with $C = (4 - 3 C^2) c_1^2 \sim 1.20$ and

$$ \tilde{V}_c = \sum_p v_p^2 \frac{\alpha_p}{\delta_b} \sqrt{\frac{\pi}{2}} \sim 70.3 \epsilon_b \sqrt{B[T]} \text{meV}; $$

(14)

Here $\hat{\epsilon}_{m,\alpha}|_K' = \hat{\epsilon}_{m,\alpha}|_{K_{-u}}$. Here $\Omega_{n}|_{-u}$, with the property $\Omega_{-n} = -\Omega_{n}|_{-u}$, stand for corrections coming from filled levels deep in the PZM. For the PZM levels they are practically linear in $u$, with $(\Omega_{0,1}) \sim (-0.646, -0.612) \tilde{V}_c/\omega_c u/2$ in the present $e$-$h$ symmetric setting; for other levels $\Omega_{n}$ are appreciable in magnitude even for $u \rightarrow 0$.

Note that interaction lifts the orbital degeneracy at zero bias $u = 0$, with $\hat{\epsilon}_1$ getting lower than $\hat{\epsilon}_0$ by

$$ (\hat{\epsilon}_0 - \hat{\epsilon}_1)|_{u=0} = \frac{1}{2} C \tilde{V}_c \equiv \epsilon_{LS}, $$

(15)

i.e., the PZM levels get orbitally Lamb-shifted [13]. Numerically, $(\hat{\epsilon}_0, \hat{\epsilon}_1, \epsilon_{LS})|_{u=0} \sim (0.72, 0.57, 0.15) \tilde{V}_c$. Let us write, for $u \neq 0$, the full $(0, 1)$ shift as

$$ \delta \epsilon = \hat{\epsilon}_0 - \hat{\epsilon}_1 \equiv (1 - \xi) \epsilon_{LS}, $$

(16)

with $\xi \equiv \{(1 - z_1) u/2 + \Omega_1 - \Omega_0\}/\epsilon_{LS} \approx u/(g^2 + 1) \epsilon_{LS}$. The spectra $(\hat{\epsilon}_0, \hat{\epsilon}_1)$ have a crossing at $\xi = u/u^{cr} = 1$ or across the critical bias

$$ u^{cr} \approx (g^2 + 1) \epsilon_{LS} \sim 1.2 \tilde{V}_c. $$

(17)

Numerically, $(\epsilon_{LS}, u^{cr}) \sim (8.3, 62) \text{meV}$ for the choice $\tilde{V}_c/\omega_c = 0.4$ or $\epsilon_b \approx 5.7$.

When the PZM levels are filled with electrons, the spectra get lower by the amount of exchange energy acting within the sector [see Eq. (12)],

$$ (\hat{\epsilon}_0, \hat{\epsilon}_1)|_{N_f=2} = (\hat{\epsilon}_0 - \epsilon_{G^{00}}, \hat{\epsilon}_1 - \epsilon_{G^{10} - G^{11}}), $$

(18)

where

$$ G^{mn} = \sum_p v_p^2 \rho_p^{m,m} \rho_p^{n,n} \approx \sum_p v_p^2 \rho_p^{m,m} \rho_p^{n,n}. $$

(19)

$G^{mn}$ is the exchange energy matrix (in Eq. (12)). Substituting the explicit values,

$$ (\epsilon_{G^{00}}, \epsilon_{G^{01}}, \epsilon_{G^{11}}, \epsilon_{G^{00:11}}) \approx \{1, \frac{1}{4} C^2, 1 - \frac{1}{2}, 0\} \tilde{V}_c, $$

(20)

yields the spectra of the filled levels,

$$ \hat{\epsilon}_0|_{N_f=2} = - \frac{1}{2} \frac{1}{\delta_b} u + \Omega_0 \frac{1}{2}(1 + \frac{1}{4} C^2) \tilde{V}_c, $$

$$ \hat{\epsilon}_1|_{N_f=2} = - \frac{1}{4} \frac{1}{\delta_b} u + \Omega_1 - \frac{1}{2}(1 + \frac{1}{4} C^2) \tilde{V}_c. $$

(21)

Here the orbital Lamb shift is enhanced and reversed in sign, $(\hat{\epsilon}_0 - \hat{\epsilon}_1)|_{N_f=2} = - (1 + \xi) \epsilon_{LS} < 0$ for $0 < \xi < 1$. Actually, the filled and empty spectra are related via $e$-$h$ conjugation [in Eq. (10)],

$$ (\hat{\epsilon}_0, \hat{\epsilon}_1)|_{N_f=2} = (- \hat{\epsilon}_0, - \hat{\epsilon}_1)|_{-u} \equiv 0. $$

(22)

The renormalized PZM sector, when either empty or filled, becomes a unique eigenstate to $O(V^C)$ of the total Hamiltonian $H_{eb} + V^C$.

Figure 1(b) depicts a typical pattern of PZM spectra $(\hat{\epsilon}_0, \hat{\epsilon}_1)|_K^{K'}$ (with $\hat{\epsilon}_0^{K'} = \hat{\epsilon}_0^{K_{-u}}$) per spin, with a crossing at $u = u^{cr}$ for empty levels in valley K and at $u = -u^{cr}$ for filled ones in valley K'. The orbital Lamb shift, upon level filling, induces a level inversion $(\hat{\epsilon}_0 > \hat{\epsilon}_1)|_{\text{empty}} \rightarrow (\hat{\epsilon}_0 < \hat{\epsilon}_1)|_{\text{filled}}$ for bias $u \in (-u^{cr}, u^{cr})$. Actually, when $e$-$h$ breaking due to $(\Delta, g_{1}, \ldots)$ is taken into account, $u^{cr}$ becomes smaller ($\sim 30 \text{meV}$ at $B = 20 T$ in valley K and far larger ($\sim 100 \text{meV}$) in $K'$ [17]. Accordingly, we focus, in what follows, on quantum phenomena related to a crossing of empty levels in valley K.]

Such a level inversion signals a level crossing or instability with filling, which actually is avoided via mixing of $n = \{0, 1\}$ levels, as noted earlier [13].

### III. LEVEL MIXING

In this section we refine an earlier analysis of orbital level mixing from a new angle. We first note that the
empty PZM sector \( n = \{0, 1\} \) (per valley and spin) to \( O(V^C) \) is described by the one-body Hamiltonian \( H^0 \) of Eq. \((11)\) with \((\epsilon_0, \epsilon_1) \) replaced by the renormalized \( (N_f = 0) \) spectra \((\epsilon_0, \epsilon_1) \) in Eq. \((14)\), we denote it as \( H^{\text{pzm}} \) and the associated fields as \( \psi = (\psi^0, \psi^1)^t \). We write the Coulomb exchange interaction acting within the PZM sector as \( V_X \) and take \( H^{\text{pzm}} + V_X \approx H^\text{eff} \) as an effective Hamiltonian that governs the sector for \( 0 \leq N_i \leq 2 \).

Let us now suppose filling the PZM levels with electrons gradually and examine how level mixing proceeds via the Coulomb interaction. To this end we rotate \( \psi = (\psi^0, \psi^1)^t \) to \( \Phi = (\Phi^0, \Phi^1)^t \) by an SU(2) matrix,

\[
\dot{\psi} = U \Phi = \left( \begin{array}{cc} c_0 & -e^{-i\phi} s_\theta \\ e^{i\phi} s_\theta & c_\theta \end{array} \right) \left( \begin{array}{c} \Phi^0 \\ \Phi^1 \end{array} \right),
\]

where \( c_\theta \equiv \cos(\theta/2) \) and \( s_\theta \equiv \sin(\theta/2) \); \((\theta, \phi)\) are real angles. We fix \( U \) so that the PZM spectra become diagonal for \( \Phi = (\Phi^0, \Phi^1)^t \) and refer to the associated levels as \( n = (0_\ell, 1_\ell) \) and their filling fractions as \( N_n = (N_0, N_1) \) (with \( 0 \leq N_n \leq 1 \). We handle the exchange interaction \( V_X \) in the Hartree-Fock (HF) approximation and cast it in the one-body form

\[
V_X^{\text{HF}} = - \sum_p v_{p}^2 \mathcal{M}^{m_\alpha a_\alpha}_{p} R^n_{0}^{m_\alpha a_\alpha},
\]

\[m_\alpha n_\alpha (U \mathcal{N} U^\dagger)^n_j g^n_{p k a},\]

where \( m, n, j, k \) run over \((0, 1); \mathcal{N} = \text{diag}(N_0, N_1)\). We thus write \( H^{\text{eff}} = H^{\text{pzm}} + V_X^{\text{HF}} \) as

\[
H^{\text{eff}} = \int d\xi \dot{\psi}^\dagger H^{\text{eff}} \dot{\psi} = \int d\xi \psi^\dagger H \Phi,
\]

\[
\dot{H}^{\text{eff}} = \left( \begin{array}{cc} a & f \\ f^t & b \end{array} \right), \quad H = U^\dagger H^{\text{eff}} U,
\]

where

\[
\begin{align*}
a &= \hat{\epsilon}_0 - (N_1 G^{G0} + N_0 G^{00}) c_\theta^2 - (N_0 G^{G0} + N_1 G^{00}) s_\theta^2, \\
b &= \hat{\epsilon}_1 - (N_1 G^{11} + N_0 G^{01}) c_\theta^2 - (N_0 G^{11} + N_1 G^{01}) s_\theta^2, \\
f &= e^{i\phi} (N_1 - N_0) G^{G00} s_\theta c_\theta + e^{i\sigma_x} (E_y + i E_x),
\end{align*}
\]

\( \text{with } G^{mn} \text{, etc., defined in Eq. }\((14)\); \((\epsilon_0, \epsilon_1)\) stand for the \( N_i = 0 \) spectra. Here we have introduced coupling to a weak uniform in-plane electric field \( \mathbf{E} = (E_x, E_y) \) to \( O(E) \), to detect an electric dipole moment induced by orbital mixing (and for another reason to be clear soon). Clearly, Eq. \((28)\) suggests setting \( \phi = \arctan(E_x/E_y) \); \( \phi \) thus controls the direction of \( \mathbf{E} \). For simplicity, we choose \( \phi = 0 \), and specifically use field \( E_y \) and measure current \( j_x \).

Let us first take a look at the case of no rotation \( \theta = 0 \) (and \( E_y = 0 \)). (i) When \( \hat{\epsilon}_1 > \epsilon_0 \), one first fills the \( n = 0 \) level. The level gap \( b - a \) increases with \( N_0 \) and then decreases with \( N_1 \), but never closes because \( G^{G0} > G^{11} > G^{01} > 0 \) holds. Filling the two levels in this way thus realizes a stable configuration. (ii) When \( \epsilon_0 > \epsilon_1 \), the \( n = 1 \) level is first filled. The level spectra \((a, b)\) then cross before \( N_i = 2 \) is reached. This means that a variation in \( \theta \) is inevitable to reach the lowest-energy configuration.

Let us therefore suppose \( \epsilon_0 > \epsilon_1 \) and try to diagonalize \( \mathcal{H} = U^\dagger H^{\text{eff}} U \). Diagonalization of \( \mathcal{H} \) is achieved for

\[
\mathcal{H}^{00} = e^{i\phi} (c_\theta^2 - s_\theta^2) - (a - b) s_\theta c_\theta \rightarrow 0,
\]

\[
\mathcal{H}^{01} = e^{i\phi} (c_\theta^2 - s_\theta^2) - (a - b) s_\theta c_\theta \\
\mathcal{H}^{11} = e^{i\phi} (c_\theta^2 - s_\theta^2) - (a - b) s_\theta c_\theta \\
\mathcal{H}^{00} = e^{i\phi} (c_\theta^2 - s_\theta^2) - (a - b) s_\theta c_\theta.
\]

Equation \((29)\), cast in the form

\[
\sin \theta \Xi + (N_1 - N_0) D \cos \theta = 2 X_E \cos \theta,
\]

fixes angle \( \theta \) as a function of filling factor \( N_i = N_1 + N_0 \). Minimization [with respect to \((\theta, \phi)\)] of the HF ground state energy also leads to the same equation.

Actually, for bilayer graphene, the combination \( D \) vanishes identically, \( D = 0 \), since \( g_0^{00} \delta^0 + g_0^{11} \delta^0 = 0 \) holds, as seen from Eq. \((11)\). Here we keep \( D \) for a later generalization, and refer to the case of bilayer graphene by showing the \( D \rightarrow 0 \) limit. For bilayer graphene we set

\[
\delta \epsilon = (1 - \varepsilon_0) \epsilon_{1s} \cos \theta \\
\Xi = \delta \epsilon - \epsilon_1, \delta G = G^{00} - G^{11}.
\]

\[
\Xi = \delta \epsilon - \epsilon_1, \delta G = G^{00} - G^{11}.
\]

Actually, for bilayer graphene, the combination \( D \) vanishes identically, \( D = 0 \), since \( g_0^{00} \delta^0 + g_0^{11} \delta^0 = 0 \) holds, as seen from Eq. \((11)\). Here we keep \( D \) for a later generalization, and refer to the case of bilayer graphene by showing the \( D \rightarrow 0 \) limit. For bilayer graphene we set

\[
\delta \epsilon = (1 - \varepsilon_0) \epsilon_{1s} \cos \theta \\
\delta G = G^{00} - G^{11}.
\]

Equation \((29)\), cast in the form

\[
\sin \theta \Xi + (N_1 - N_0) D \cos \theta = 2 X_E \cos \theta,
\]

Note first that, for \( E_y \neq 0 \), \( \sin \theta = 0 \) is not a solution to Eq. \((11)\). This means that, as \( N_i \) is increased from \( 0 \) to \( 2 \), \( \theta \) lies in either domain \( 0 < \theta < \pi \) or \( -\pi < \theta < 0 \). In particular, for \( N_i \rightarrow 0 \), Eq. \((11)\) yields

\[
\theta \equiv \delta \theta E = 2 X_E / \delta \epsilon \quad \text{(mod } \pi),
\]

while, for \( N_i \rightarrow 2 \), one finds

\[
\theta \equiv -\delta \theta E = -2 X_E / (\delta G - \delta \epsilon) \quad \text{(mod } \pi);
\]

\[
\delta \theta E \rightarrow \frac{2 (X_E / \epsilon_{1s})}{1 + \Xi}. \]

Actually, the \( \theta > 0 \) and \( \theta < 0 \) solutions for \( U \) are related by a unitary transformation, \( U|_{\theta \rightarrow \phi} = Y U Y^{-1} \) with \( Y = e^{i\pi \sigma_z / 2} i \sigma_3 \). This fact reflects the invariance of the system under a rotation by angle \( \pi \) of coordinates \( \text{or } (x, y) \rightarrow - (x, y) \), as seen from the associated change of \( H^{\text{eff}} \) in Eq. \((29)\). \( Y H^{\text{eff}} Y^{-1} = H^{\text{eff}} |_{\theta \rightarrow - \phi} \).

U is thus naturally defined for \( -\pi \leq \theta \leq \pi \). In view of the anti-periodicity \( U|_{\theta + 2 \pi} = - U|_{\theta} \), one can even extend \( U \) over the full line \(-\infty < \theta < \infty\).
For a given angle $\theta$, the level spectra ($\mathcal{H}^{00}, \mathcal{H}^{11}$) are cast in the following two equivalent forms

$$
\hat{\epsilon}_0 = \hat{\epsilon}_1 - N_1 G^{01} - N_0 G^{00} - \Delta s_0^2 + (s_0/c_0) X_E, \\
\hat{\epsilon}_1 = \hat{\epsilon}_0 - N_1 G^{11} - N_0 G^{01} - \Gamma s_0^2 - (s_0/c_0) X_E,
$$

and

$$
\hat{\epsilon}_0 = \hat{\epsilon}_1 - N_1 G^{01} - N_0 G^{11} + \Gamma s_0^2 + (c_0/s_0) X_E, \\
\hat{\epsilon}_1 = \hat{\epsilon}_0 - N_1 G^{00} - N_0 G^{01} - \Gamma s_0^2 - (c_0/s_0) X_E,
$$

where

$$
\Lambda = (N_1 - N_0) D \xrightarrow{D \to 0} 0, \\
\Gamma = (N_1 - N_0)(\delta G - D) \xrightarrow{D \to 0} 2(N_1 - N_0) \epsilon_{Ls}.
$$

See Appendix A for a derivation of these spectra.

Equation (35) shows how the spectra ($\hat{\epsilon}_0, \hat{\epsilon}_1$) deviate from the $\theta = 0$ spectra (of no rotation) as $\theta$ grows from zero. In contrast, Eq. (36) shows how they approach, as $\theta \to \pm \pi$ or $c_0 \to 0$, the $\theta = \pm \pi$ spectra, which, as $N_1 \to 2$, attain the filled-level spectra in Eq. (15).

$$(\hat{\epsilon}_0, \hat{\epsilon}_1)|_{\theta \to \pm \pi} = (\hat{\epsilon}_1|_{N_1 = 2}, \hat{\epsilon}_0|_{N_0 = 2}).$$

Thus the empty $n = (0, 1)$ levels, when filled, turn into the $n = (1, 0)$ levels.

Figure 2(a) depicts, for bilayer graphene at $B = 20$ T, how $(s_0)^2 = \sin^2(\theta/2)$ grows as a function of filling factor $N_1$ for certain values of bias $u$; there Eq. (31) is numerically solved for $\theta$, with the choice $X_E/\epsilon_{Ls} = 0.01$ and $V_c/\omega_c = 0.4$. $\theta$ starts to rise around $N_1 \sim \frac{1}{2}(1 - u/w^\text{cr})$.

Figure 2(b) illustrates how PZM spectra ($\hat{\epsilon}_0, \hat{\epsilon}_1$) avoid a crossing via orbital mixing as they evolve with increasing $N_1$. A sizable gap arises at half-filling $N_1 = 1$, with ($\hat{\epsilon}_0, \hat{\epsilon}_1)|_{N_1 = 1} = (\hat{\epsilon}_0 - G^{01}, \hat{\epsilon}_0 - G^{00})$ for $X_E \to 0$. Also depicted in Fig. 2(c) is the profile of electric dipole moment induced by orbital mixing, calculated by numerically differentiating the spectra with respect to $E_y$.

Figure 2(d) shows how the PZM spectra evolve with bias $u$ for the empty, half-filled and filled sector ($N_1 = 0, 1, 2$). Dotted lines refer to empty levels. In orbital mixing, both levels $\{0_1, 1_0\}$ get shifted with filling $N_1 = 2$. This is in sharp contrast to the case of Coulomb-enhanced spin splitting, depicted in Fig. 2(e).

It is seen from Eqs. (38) and (39) that the level spectra at angle $\theta$ and at $\pi - \theta$ have reciprocity of the form

$$
(\hat{\epsilon}_0, \hat{\epsilon}_1)|_{\theta \to \pi - \theta} = (\hat{\epsilon}_1, \hat{\epsilon}_0)|_{N_1 \to N_0, N_0 \to N_1, -X_E}.
$$

This reciprocity derives from the invariance of the basic Hamiltonian $\mathcal{H}^{\text{eff}}$ [in Eq. (27)],

$$
\mathcal{H}^{\text{eff}}|_{\theta \to \pi - \theta, N_0 \to N_1, -X_E} = \mathcal{H}^{\text{eff}},
$$

under simultaneous replacement $\theta \to \pi - \theta$ (i.e., $s_\theta \leftrightarrow c_\theta$), $N_0 \leftrightarrow N_1$ and $X_E \to -X_E$.

Equation (39) implies, in particular, that the $\theta = \pi$ spectra ($\hat{\epsilon}_0, \hat{\epsilon}_1$)|$_{\theta \to \pi}$ [in Eq. (35)] are equal to the $\theta = 0$ spectra ($\hat{\epsilon}_0, \hat{\epsilon}_1$)|$_{\theta \to 0}$ of Eq. (35) with $N_1 \leftrightarrow N_0$ and $X_E \to -X_E$.

$E_y \to -E_y$. Interchanging $N_1$ and $N_0$ is to adopt, for a given $N_1 = N_1 + N_0$, the filling sequence of the $u > u^\text{cr}$ case (of $\delta \theta < 0$ and no rotation). From this follows an important observation: The $\theta = \pi$ spectra with $u \to u^\text{cr}$ upward are equal to the $\theta = 0$ spectra with $u \to u^\text{cr}$ downward. The PZM spectra, when regarded as a function of $N_1$ and bias $u$, are thus smoothly connected across $u = u^\text{cr}$; we will see an example later.

To see how $\theta$ depends on filling $N_1$ explicitly (apart from its sign) one can simply set $E_y \to 0$ in Eq. (31). One then finds either $\sin \theta = 0$ or, if $\sin \theta \neq 0$,

$$
\Xi + (N_1 - N_0) D \cos \theta = 0,
$$

which yields

$$
\sin^2 \theta = \frac{N_1 \delta G - \delta \hat{\epsilon} - (N_1 - N_0) D}{(N_1 - N_0)(\delta G - 2D)}. \tag{42}
$$

Note that $s_\theta^2 = 0$ for $N_1 = N_1^-$ and $s_\theta^2 = 1$ (i.e., $\theta = \pm \pi$) for $N_0 = N_0^+$, with

$$
N_1^- \equiv (\delta \hat{\epsilon} - N_0 D)/(\delta G - D) \xrightarrow{D \to 0} 
\frac{1}{2}(1 - \xi), \\
N_0^+ \equiv (\delta \hat{\epsilon} - N_1 D)/(\delta G - D) \xrightarrow{D \to 0} 
\frac{1}{2}(1 - \xi). \tag{43}
$$
In terms of these Eq. (42) is neatly expressed as

\[ s_0^2 = \frac{N_1 - N_1^-}{N_1 - N_0} f_D, \]

where \( f_D \equiv (\delta G - D)/(\delta G - 2D) \). When \( \delta G > 0 \), filling of the empty PZM sector starts with the \( 1_\theta \) level. The angle \( \theta \) shows different behavior in the following three domains,

(i) \( 0 \leq N_1 \leq N_1^- \), \( \theta = 0; N_0 = 0 \),
(ii) \( N_1^- \leq N_1 \leq 1 + N_0^+ \), \( s_0^2 = 0 \rightarrow 1 \),
(iii) \( 1 + N_0^+ < N_1 \leq 2 \), \( ||\theta| = \pi; N_1 = 1 \). (45)

\( \theta \) remains 0 as the \( 1_\theta \) level is filled over domain (i), and rises to \( \pi \) (or \(-\pi\)) through domain (ii), retaining \( s_0 = 1 \) thereafter over (iii). As seen from Fig. 2(a), the effect of \( X_E \times E_y \) is noticeable \( \boxed{[30]} \) only near the boundaries of domain (ii).

Empty PZM levels \( n = \{0, 1\} \) have a crossovers when one sweeps bias \( u \) across \( u^c \). It is enlightening to see how they avoid a crossovers when one of them is partially filled. Let us take \( N_1 = N_1^+ < 0.5 \) and try to solve Eq. (42) for \( \theta \), with \( X_E/x_{1a} = 0.01 \) chosen. As seen from Fig. 3, \( \theta \) starts to rise above \( u^c \sim 1 - 2N_1 \) and reaches \( \pi \) for \( u \geq u^c \), with a rapid rise near \( u \sim u^c \) for \( N_1 \ll 1 \). The associated spectra \( (\epsilon_{0u}, \epsilon_{1s}) \) always stay apart, and the \( u < u^c \) spectra \( (\epsilon_{0u}, \epsilon_{1s}) \) are smoothly connected to the \( u \sim u^c \) spectra \( (\epsilon_{0u}, \epsilon_{1s}) \) for \( u \geq u^c \). In this way, a level gap generally develops with filling via interaction. In practice, however, for small filling \( N_1 \ll 1 \) an emerging small gap will be readily washed away by disorder and finite temperature. One will then observe a collapse of the quantized conductance around \( u \sim u^c \), noticing as if a level crossing had taken place.

We have so far handled mixing of PZM levels in bi-layer graphene. It will be clear now that an inversion of spectra, such as \( (\epsilon_m > \epsilon_n) \) (empty) \( \rightarrow (\epsilon_m < \epsilon_n) \) (filled), is induced by a difference in orbital exchange energy that generally has the property \( G_{mn} > G_{nm} > G_{mi} > 0 \) for \( n > m \geq 0 \). The present analysis is equally applicable to such a general case of orbital mixing by simply replacing orbital labels \((0,1) \rightarrow (m,n) \) with \( m < n \).

### IV. NON-ABELIAN BERRY’S PHASE

In this section we wish to clarify algebraic features of orbital-mixing phenomena. Let us first note that, once \( H = U^\dagger H^{\text{eff}} U \) is diagonalized, \( U \) and \( H \) are fixed as a function of filling factor \( N_1 = N_1 + N_0 \). Suppose now that we start filling the empty PZM sector by increasing \( N_1 \) gradually in time, i.e., we set \( N_1 \rightarrow N_1(t) \), and ask how the sector evolves. The eigenmodes of \( H^{\text{eff}} \) are merely the \( N_1 \rightarrow N_1(t) \) in each instant are thereby written as \( \psi^{(n)}(t) = U |N_1(t)\psi^{(n)}(t) = U(t)\psi^{(n)}(t) \) with \( \Phi^{(0)} = (1, 0)^t \) and \( \Phi^{(1)} = (0, 1)^t \), and have nondegenerate spectra \( \{H_{00}^{\text{eff}}, H_{11}^{\text{eff}}\} \). The time evolution of the PZM levels is best clarified by referring to the Lagrangian (or action)

\[ L = \int dt dy [\dot{\psi}^\dagger (i\partial_t - H^{\text{eff}})\psi]. \]

Rewriting \( L \) in terms of \( \Phi = U^\dagger \hat{\psi} \) yields

\[ L = \int dt dy \Phi^\dagger [i\partial_t - H + i(U^\dagger \partial_t U)] \Phi, \]

which describes how the field \( \Phi = (\Phi^{(0)}, \Phi^{(1)}) \), expanded in instantaneous eigenmodes \( \{\Phi^{(0)}, \Phi^{(1)}\} \), evolves in time. It tells us that the field \( \Phi \) and associated \( (0_1) \) levels have excitation spectra \( (\epsilon_{0u}, \epsilon_{1s}) \) over the instantaneous ground state that evolves along a nontrivial path of mixing [specified by \( U(t) \)] in the \( \{\psi^{(0)}, \psi^{(1)}\} \) space.

Here we notice a non-Abelian Berry phase \[29\] \( \mathcal{A} = -i(U^\dagger \partial_t U) = i(\partial_t U^\dagger)U \), or the SU(2) connection

\[ \mathcal{A} = -i(U^\dagger \partial_t U = i(\partial_t U^\dagger)U \), \]

In terms of Pauli matrices \( \sigma_a \), \( \mathcal{A}_a = \sum_{a=1}^3 A_a^a \sigma_a/2 \), with

\[ A_0^a = (\sin \phi \cos \phi, 0), \]
\[ A_1^a = (\cos \phi \sin \theta \sin \phi, \sin \phi \sin \theta \cos \phi, -1 - \cos \theta). \]

Formally the rotation \( U^\dagger = U^\dagger(t) \) is written as a time-ordered (or path-ordered \( \mathcal{P} \)) integral of \( \mathcal{A} \),

\[ U^\dagger (t) = \mathcal{P} \exp \left[ -i \int_0^t dt \mathcal{A} \right] U^\dagger(0). \]

For \( \phi = 0 \), in particular, \( A_0^a \rightarrow (0, -1, 0) \) and

\[ U^\dagger (t) \overset{\phi = 0}{=} e^{i\phi \sigma_2}/2 = c_0 \mathbf{1} + is_0 \sigma_2 \]

is fixed by a net adiabatic change of \( \theta = \theta |N_1(t) \) alone. The SU(2) gauge field \( \mathcal{A}_a \), associated with filling of the PZM levels, derives from interaction \( V \) and resides in the space of parameters \( (\theta, \phi) \), through which one can adiabatically change the filling factor \( N_1(t) = N_1(t) + N_0(t) \), interlayer bias \( u(t) \), electric field \( E(t) \), etc.

Let us now recall how \( \theta \) behaves in domains (i)-(iii) of Eq. (45) and reexamine the evolution of the PZM sector.
(for δt > 0 and u < u^{cr}). To choose the sign of θ we start filling the empty sector by gradually turning on a weak field E_y > 0 in domain (i), and turn it off later when the sector is filled. The angle θ then rises from 0 to π as N_f = 0 → 2 over time interval T, so that

\[ U^{\dagger}|_{t=0}=1 \rightarrow U^{\dagger}|_{t=T}=e^{i\pi\sigma_z/2}= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_2. \]

The instantaneous eigenmodes Φ = (Φ^0, Φ^1)^t thereby evolve as mixtures of (ψ^0, ψ^1) without a crossing,

\[ \Phi^{\text{empty}}|_{\theta=0}=(\psi^0, \psi^1)^t \rightarrow \Phi^{\text{filled}}|_{\theta=\pi}=(\psi^1, -\psi^0)^t, \]

Thus the presence of active (i.e., interaction-induced) orbital level mixing is characterized by θ = π and tr[U] = 0.

\[ V. \text{ TRILAYERS} \]

Trilayer graphene supports 4 × 3 = 12 PZM levels with a three-fold orbital degeneracy. As discussed theoretically [4, 48, 49] and observed experimentally [42, 43], the Landau-level spectra and electronic properties of trilayers strongly depend on the stacking order, such as ABA and ABC stackings. The orbital degeneracy is again lifted by the Coulomb interaction and the orbital Lamb shift leads to orbital mixing, as noted earlier [41]. In this section we summarize and refine the result in the light of the present framework of level mixing.

The ABC-stacked trilayer is a chiral generalization [4] of bilayer graphene and the zero-energy modes residing primarily in outer layers show a degeneracy in orbitals n = (0, 1, 2) per spin and valley. The one-body spectra \( \epsilon_n, \epsilon_{n+1} \) deviate from zero energy by a symmetric interlayer bias u, with slightly different gradients, and the two valleys are related, e.g., as \( \epsilon_{n}|K'| = \epsilon_{n}|K_u \) per spin. The orbital Lamb-shift corrections read [41], e.g.,

\[ (\epsilon_{0}^{LA}, \epsilon_{1}^{LA}, \epsilon_{2}^{LA}) \approx B=10T \ (0.888, 0.777, 0.641) \bar{\nu}_e \]

numerically, with only the leading band parameter g = γ_{11}/ω ≈ 3.41 kept at B = 10 T. The PZM spectra \( \hat{\epsilon}_n = \epsilon_n + \epsilon_{n}^{LA} \) are ordered as \( \hat{\epsilon}_0 > \hat{\epsilon}_1 > \hat{\epsilon}_2 > 0 \) for empty levels at zero bias u = 0 while they change sign for filled levels so that 0 > \hat{\epsilon}_2 > \hat{\epsilon}_1 > \hat{\epsilon}_0 at \ N_f = 3. \ This signals the presence of orbital mixing upon level filling.

To study level mixing let us rotate, as in the bilayer case, the PZM sector \( \psi = (\psi^0, \psi^1, \psi^2)^t \) to \( \hat{\psi} = (\psi^0, \psi^1)^t \) thus flips sign,

\[ \Phi^{\text{empty}}|_{\theta=0} \rightarrow \Phi^{\text{empty}}|_{\theta=\pi} = \hat{\psi}, \]

simply because \( \hat{\psi} \) has made a 2π rotation relative to Φ in the spinor space.

Case [II]: Turn on a weak field (reversed in sign) E_y turned on as before. One then comes back to the initial and final configurations are physically the same although they differ in assignment of \( \psi \) to Φ, 3.5

\[ \Phi^{\text{empty}}|_{\theta=\pi} = (\psi^0, \psi^1)^t \rightarrow \Phi^{\text{empty}}|_{\theta=\pi} = (\psi^1, -\psi^0)^t. \]

The initial and final configurations are physically the same although they differ in assignment of \( \psi \) to Φ, 3.5

\[ V. \text{ TRILAYERS} \]

Trilayer graphene supports 4 × 3 = 12 PZM levels with a three-fold orbital degeneracy. As discussed theoretically [4, 48, 49] and observed experimentally [42, 43], the Landau-level spectra and electronic properties of trilayers strongly depend on the stacking order, such as ABA and ABC stackings. The orbital degeneracy is again lifted by the Coulomb interaction and the orbital Lamb shift leads to orbital mixing, as noted earlier [41]. In this section we summarize and refine the result in the light of the present framework of level mixing.

The ABC-stacked trilayer is a chiral generalization [4] of bilayer graphene and the zero-energy modes residing primarily in outer layers show a degeneracy in orbitals n = (0, 1, 2) per spin and valley. The one-body spectra \( \epsilon_n, \epsilon_{n+1} \) deviate from zero energy by a symmetric interlayer bias u, with slightly different gradients, and the two valleys are related, e.g., as \( \epsilon_{n}|K'| = \epsilon_{n}|K_u \) per spin. The orbital Lamb-shift corrections read [41], e.g.,

\[ (\epsilon_{0}^{LA}, \epsilon_{1}^{LA}, \epsilon_{2}^{LA}) \approx B=10T \ (0.888, 0.777, 0.641) \bar{\nu}_e \]

numerically, with only the leading band parameter g = γ_{11}/ω ≈ 3.41 kept at B = 10 T. The PZM spectra \( \hat{\epsilon}_n = \epsilon_n + \epsilon_{n}^{LA} \) are ordered as \( \hat{\epsilon}_0 > \hat{\epsilon}_1 > \hat{\epsilon}_2 > 0 \) for empty levels at zero bias u = 0 while they change sign for filled levels so that 0 > \hat{\epsilon}_2 > \hat{\epsilon}_1 > \hat{\epsilon}_0 at \ N_f = 3. \ This signals the presence of orbital mixing upon level filling.

To study level mixing let us rotate, as in the bilayer case, the PZM sector \( \psi = (\psi^0, \psi^1, \psi^2)^t \) to \( \hat{\psi} = (\psi^0, \psi^1)^t \) thus flips sign,

\[ \Phi^{\text{empty}}|_{\theta=\pi} = (\psi^0, \psi^1)^t \rightarrow \Phi^{\text{empty}}|_{\theta=\pi} = (\psi^1, -\psi^0)^t. \]

The initial and final configurations are physically the same although they differ in assignment of \( \psi \) to Φ, 3.5
(Φ0, Φ1, Φ2)\textsuperscript{T} by an SO(3) matrix \( U, \hat{\psi} = U \Phi \), and try to diagonalize the HF effective Hamiltonian \( H_{\text{eff}} \) (taken to be a real symmetric matrix). Previously we wrote \( U \) as a product of three rotations and fixed it numerically as a function of filling factor \( N_1 \) at zero bias \( u = 0 \). It is illuminating to cast the result in the polar form

\[
U = e^{i\Theta \cdot n \cdot t} = e^{i\Theta n \cdot t},
\]

where \( t = (t_0, t_1, t_2) \) stand for the spin-1 generators \( (t_0) = e^{i e_{abc}} \) with the totally antisymmetric tensor \( e_{abc} \) and \( e^{012} = 1 \); real angles \( \Theta = (\chi_0, \chi_1, \chi_2) = (\Theta n) \) are decomposed into the magnitude \( \Theta \equiv |\Theta| \) and a unit vector \( n = (n_0, n_1, n_2) \); \( n \cdot t = n_0 t_0 \). Note that \( \chi_0 \) mixes \( n = (1, 2), \chi_1 \) mixes \( (0, 2), \) etc. Some useful formulas are

\[
e^{i\Theta n \cdot t} = 1 + (\cos \Theta - 1) P + i(n \cdot t) \sin \Theta, \\
\text{tr}[e^{i\Theta n \cdot t}] = 1 + 2 \cos \Theta,
\]

where \( P = (n \cdot t)^2 \) is a projection operator, \( P^2 = P \) and \( (n \cdot t)P = (n \cdot t) \); \( P_{ab} = \delta_{ab} - n_0 n_b \).

Figure 5 illustrates how the angle \( \Theta \) and direction \( n \) change with filling factor \( N_1 \). \( \Theta \) rises from zero to \( \pi \) over the interval \( 0.51 \lesssim N_1 \lesssim 2.51 \) and \( n \) lies around \( n_{\Theta=\pi} = (1, 0, 1)/\sqrt{2} \). It is essential that the three levels cooperate, with the associated SO(3) Berry phase \( A_{\Theta} \approx n \cdot t \). At \( N_1 = 3 \) and \( \Theta = \pi \),

\[
U = e^{i\pi t \cdot n_{\Theta=\pi}} = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad \text{tr}(U) = -1. 
\]

(62)

Upon filling, the eigenmodes \((\Phi_0, \Phi_1, \Phi_2)\) thus evolve from \((\psi^0, \psi^1, \psi^2)|_{N_1=0}\) to \((\psi^0, -\psi^1, \psi^2)|_{N_1=3}\) without a crossing, as seen from Fig. 5(b).

There is another solution that differs from one shown in the figure by signs, \((n_0, n_1, n_2) \rightarrow (-n_0, n_1, -n_2)\). It is related to \( U \) by a unitary transformation, \( U_{-n_0, n_1, -n_2} = \mathcal{Y} U_{n_0, n_1, n_2} \) with \( \mathcal{Y} = e^{i\pi t_1} = \text{diag}[-1, 1, -1] \), and reflects again the invariance of the system under a spatial \( \pi \) rotation, \( x \rightarrow -x \). It is enlightening to interpret \( U_{-n_0, n_1, -n_2} \) as a rotation by negative angle \( \Theta < 0 \) about the axis \( n' = (n_0, -n_1, n_2) \). Then \( U = e^{i\Theta n' \cdot t} \), as a function of \( N_1 \), is naturally defined for \( -\pi \leq \Theta \leq \pi \), and even for the full line \( -\infty < \Theta < \infty \) if one notes that \( U \) has period \( 2\pi \) in \( \Theta \). One can also control the sign of \( \Theta \) by use of a weak in-plane field \( E_0 \) [41]. It is clear now that \( U \) acts as a path-dependent non-Abelian phase factor when one controls \((\Theta, n)\) via adiabatic changes of external parameters \((N_1, E, u, \cdots)\), as in Fig. 4 of the bilayer case.

Previously \( U_{\Theta=\pi} \) was obtained as a product of three \( \pi/2 \) rotations, \( U = e^{-i(\pi/2)\alpha -i(\pi/2)\beta -i(\pi/2)\gamma} \). A single \( \Theta = \pi/2 \) rotation, e.g., \( e^{i(\pi/2)\alpha} = 1 \oplus i\delta_2 \), consists of a \( \Theta = \pi \) rotation of \((\psi^1, \psi^2), \psi^0 \) left intact. Such a \([\Theta] = \pi/2 \) rotation has been encountered in a study [41] of \( ABA \)-stacked trilayer graphene. The \( ABA \) trilayer accommodates \([44]\) monolayer-like and bilayer-like subbands, and has the PZM levels specified by orbital labels such as \( n = (n_0, 1\pm, 1) \) in one valley and \( n = (0\pm, 1) \) in another valley. It turns out that Coulomb exchange interactions mainly act between \((0, 1-), \) leaving \( 1+ \) rather isolated; analogously for \((1, 0-) \) and \( 0+ \). This explains why \( \Theta = \pi/2 \) rotations are responsible for mixing of PZM levels in the \( ABA \) trilayer. In this way, indices \( \text{tr}(U|_{\Theta=\pi}) = -1 \) and \( \text{tr}(U|_{\Theta=\pi/2}) = 1 \) clearly distinguish \( ABC \) and \( ABA \) trilayers in their character of orbital mixing.

VI. EVOLUTION AND CROSSING OF MANY-BODY STATES

Bilayer graphene has four renormalized PZM sectors of valley \((K, K') \times \text{spin} (\uparrow, \downarrow)\). Each sector, when empty or filled, becomes an eigenstate to \( O(V' C) \) of the total Hamiltonian \( H_{1b} + V' C \), as we have noted. Such empty and filled sectors do not mix by exchange interaction to \( O(V' C) \), unless there is a degeneracy (i.e., unless they cross). In the light of this picture, we discuss in this section what the \( \nu = 0 \) ground state is like when orbital splitting \( \epsilon_{ls} \) and spin splitting (with Zeeman energy \( \mu_2 \equiv g^* \mu_B B \sim 0.12 B[T] \)) are taken into account. We start with the four empty PZM sectors that constitute the unique ground state at total filling factor \( \nu = -4 \), and consider filling them with electrons gradually.

Whenever nonzero bias \( u > 0 \) induces a sizable valley gap \( \sim u \), the \( \nu = 0 \) ground state is certainly realized as a valley-polarized one with \((1^K, 0^K) + (1^{K'}, 0^{K'}) \) filled (in obvious notation) and of total energy (per electron)

\[
\epsilon^{(v)} = 2(\hat{\epsilon}_0 + \hat{\epsilon}_1)|_{N=2},
\]

which gets lower with increasing bias \( u \).

For small bias \( u \sim 0 \), spin splitting will become important. See Fig. 6. Figure 6(a) depicts the empty level spectra of the \( \nu = -4 \) ground state for \( \epsilon_{ls} \lesssim \mu_2 \), as is normally the case. At \( u \sim 0 \), \((1^K, 1^{K'}) \) are lower than others (for both \( \epsilon_{ls} \lesssim \mu_2 \) and \( \epsilon_{ls} > \mu_2 \)). Accordingly, for \( u \sim 0 \), the \( \nu = -4 \) state [in 6(a)], upon filling \((1^K, 0^{K'}) \) and \((1^{K'}, 0^K) \) in sequence or in some other order, will evolve into a spin-polarized \( \nu = 0 \) ground state [in 6(b)]
of total energy

\[ \epsilon^{(s)} = (\epsilon_0 + \epsilon_1)|_{N_l=2} + (\epsilon_0 + \epsilon_1)|_{N_l=2} - 2\mu_Z, \]

which barely depends on \( u \).

Of these two \( \nu = 0 \) candidates the spin-polarized state is generally favored for \( u \sim 0 \), as seen from

\[ \epsilon^{(\nu)} - \epsilon^{(s)} = 2(\mu_Z - \kappa|u|) \approx 2(\mu_Z - \lambda u), \]

where \( \kappa|u| = (1 + z_1)u/2 - \Omega_0 - \Omega_1 \approx \lambda u \) and \( \lambda = O(1) \). The \( \nu = 0 \) ground state, if formed as a spin-polarized one [in 6(b)] at \( u \sim 0 \), will eventually evolve into a valley-polarized state [in 6(c)] as \( u \) is increased. Let us consider how this transition takes place. Figure 6(d) depicts the filled spectra of the spin-polarized state with those of the other superposed. Figure 6(e) shows similar spectra for the case \( \mu_Z > \epsilon_L \) in high field \( B \). Let us first take a look at the latter. There, as \( u \) is increased, the valley-polarized virtual state comes down in energy and, at first, filled \( K^\nu \) meets \( 0^K \). At this point of degeneracy, \( 1^K' \) has a chance to turn into filled \( 0^K_1 \), but this is not possible because filled \( 1^K' \) has to first mix with empty \( 0^K_1 \) which lies far above in the spectra.

Next, filled \( 0^K_1 \) meets \( 0^K \) in the figure. At this degeneracy, filled \( 0^K_1 \) can readily turn into filled \( 0^K_1 \) via a global rotation in the valley-spin space. Note that \( \rho^{0,0:K' = K} = \rho^{0:0:K = K} = 1 \) so that, within the \( n = 0 \) sector, the Coulomb interaction is invariant under rotations in valleys and spins. Thus there is no extra cost of energy in making a rotation \( (0^K_1|_{\text{empty}} , 0^K_1|_{\text{filled}}) \xrightarrow{U} (0^K_1|_{\text{empty}} , 0^K_1|_{\text{filled}}) \), with a non-Abelian Berry phase \( U \), and \( \text{tr}[U] = 0 \).

Such a rotation takes place across the critical bias

\[ u^{ct}_0 = \mu_Z/\lambda_0, \]

with \( \lambda_0 = 1 - 2\Omega_0/u \sim 20T \) and \( \lambda = 0.65 \bar{V}_c/\omega_c \). See Appendix B for details. Similarly, filled \( 1^K' \) turns into filled \( 1^K \) with little cost of energy across the second critical bias

\[ u^{ct}_1 = \mu_Z/\lambda_1 > u^{ct}_0, \]

and continues for \( u > u^{ct}_1 \). For \( u \in (u^{ct}_0, u^{ct}_1) \) the ground state is polarized in both valley and spin; this intermediate state differs in structure from one discussed earlier in Refs. [13, 16]. It is clear from Fig. 6(d) that the transition follows the same steps for the case \( \epsilon_L \approx \mu_Z \) as well. Inclusion of weak \( e\hbar \) breaking \( (\Delta, \gamma_4, \ldots) \) also leaves this two-step picture qualitatively intact.

An observable signature of such transitions is the following: With increasing bias \( u \), the quantum Hall effect will survive as long as the ground state and competing virtual state retain an appreciable energy gap. Incompressibility will be lost and conductance \( \sigma_{xx} \) will rise from zero only when bias \( u \) lies around these critical values \( u^{ct}_0 \) and \( u^{ct}_1 \). It is clear, on interchanging valleys \( K \leftrightarrow K' \), that negative bias \( u < 0 \) also leads to the same sequence of transition.

Actually, early transport experiments [20, 22] observed a collapse of the \( \nu = 0 \) quantum Hall state at two distinct (positive/negative) values of electric field \( \propto u \), and later capacitance measurements [23, 24] in higher magnetic field \( B \) detected it at four such values of \( u \). The transition sequence in Eq. (68) appears consistent with one inferred from layer-sensitive capacitance measurements of Hunt et al. [25].

VII. SUMMARY AND DISCUSSION

Characteristic to few-layer Dirac electron systems in a magnetic field is a multiplet, at the LLL, of PZM levels nearly degenerate in orbitals, valleys and spins. Their spectra are sensitive to interactions and external perturbations, and, in particular, the orbital Lamb shift inevitably induces a level inversion between the empty and filled levels in a way governed by \( e\hbar \) symmetry.

In the present paper we have examined how those PZM levels evolve with increasing filling and external bias \( u \) under many-body interactions, and have seen that they generally avoid a crossing via level mixing which is governed by a non-Abelian Berry’s phase (factor) \( U \). This Berry’s phase derives from interactions, and encodes, in
the form of trace $\text{tr}(U)$, how a nearly degenerate system responds to adiabatic external changes, such as the filling factor, electric and magnetic fields. Its path dependence, in particular, reveals algebraic features underlying general Landau-level crossing/mixing phenomena. Our basic picture of level mixing is also applicable to evolution of many-body ground states with sweeping external perturbations, as examined in Sec. VI for the $\nu = 0$ ground state in bilayer graphene.

Landau-level crossing/mixing phenomena deserve serious attention as a platform to explore, both theoretically and experimentally, many-body physics. Our focus has so far been on mixing of PZM levels themselves. Crossings of PZM levels with other higher levels, as observed in ABA trilayer graphene [43], deserve equal attention, we remark, although a close look into their many-body features is left here for future study.

ACKNOWLEDGMENTS

This work was supported in part by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture of Japan (Grant No. 21K03534).

Appendix A: Rotated level spectra

In this appendix we outline the derivation of the level spectra in Eqs. (35) and (36). The diagonal elements of $\mathcal{H} = U^\dagger H^{\text{eff}} U$ in Eq. (27) are written as

$$
\mathcal{H}^{00} = a c^2_0 + b s^2_0 + 2F s_0 c_0,
$$

$$
\mathcal{H}^{11} = a s^2_0 + b c^2_0 - 2F s_0 c_0,
$$

with $F \equiv (N_1 - N_0) G^{00} s_0 + X_E$ and $X_E = c_1 c_2 E_q/\sqrt{2}$. Note parametrization in Eq. (30) for direct calculations. The spectra are thereby rewritten as

$$
\mathcal{H}^{00} = \hat{\epsilon}_0 - N_1 G^{01} - N_0 G^{00} - X^0,
$$

$$
\mathcal{H}^{11} = \hat{\epsilon}_0 - N_1 G^{00} - N_0 G^{01} - X^1,
$$

with

$$
X^0 = \Xi s^2_0 + 2s_0 c_0 (s_0 c_0 \Lambda - X_E),
$$

$$
X^1 = \Xi s^2_0 - 2s_0 c_0 (s_0 c_0 \Lambda - X_E),
$$

where $\Lambda = (N_1 - N_0) D$

On the other hand, $\mathcal{H}^{10} = 0$ [Eq. (29)] implies the relation $\Xi = (c^2_0 - s^2_0) (-\Lambda + X_E/s_0 c_0)$. Substituting this into Eq. (A3) yields

$$
X^0 = \Lambda s^2_0 - (s_0/c_0) X_E,
$$

$$
X^1 = -\Lambda c^2_0 + (c_0/s_0) X_E.
$$

Note that $X^0 + X^1 = \Xi$, which then reads

$$
\delta \Xi \equiv \hat{\epsilon}_0 - \hat{\epsilon}_1 = (N_1 s^2_0 + N_0 s^2_0) \delta G + X^0 + X^1.
$$

On replacing $\hat{\epsilon}_0 \rightarrow \hat{\epsilon}_1 + \delta \hat{\epsilon}$ in Eq. (A2), the spectra are cast in two equivalent forms in Eqs. (35) and (36).

Appendix B: Global mixing among PZM levels

In this appendix we examine how global rotations $0^0 \rightarrow \leftarrow 0^1$ and $1^0 \rightarrow \leftarrow 1^1$, posed in Sec. VI, proceed via exchange interaction. Let us start with the $n = 0$ orbital modes, and try to rotate a pair of (empty, filled) fields $(\hat{\psi}_{0}^{K}, \hat{\psi}_{1}^{K'})$ to $(\hat{\Phi}_{0}, \hat{\Phi}_{1})$ by a unitary matrix $U(\theta)$, as in Eq. (29). As verified readily, the associated HF interaction $V^H_X$ takes a simple form

$$
V^H_X = -G^{00} (N^1 \mathcal{R}_{\text{eff}, 0} + N^e \mathcal{R}_{\text{ee}, 0})
$$

in terms of $(\hat{\Phi}_{0}, \hat{\Phi}_{1})$ with filling fractions $(N^e, N^1)$ and charge operators $\mathcal{R}_{\text{eff}, 0} = \int d\theta \hat{\Phi}_{0}^{\dagger} \hat{\Phi}_{1}$, etc. Setting $(N^e, N^1) \rightarrow (0, 1)$ shows that global valley$\times$spin rotations of the filled $n = 0$ level $(\sim \hat{\Phi}_{1})$ require no extra cost of Coulombic energy.

The one-body terms with spectra $\hat{\epsilon}_0^{K'} = \hat{\epsilon}_0^{K} + \mu_Z/2$ and $\hat{\epsilon}_0^{K'} = \hat{\epsilon}_0^{K} - \mu_Z/2$ are combined with $V^H_X$ to yield the effective Hamiltonian for the rotated field,

$$
\mathcal{H}^{\text{eff}} = \{ \epsilon_f(\theta) - G^{00} \} (\mathcal{R}_{\text{eff}, 0} + \epsilon_e(\theta) \mathcal{R}_{\text{ee}, 0})
$$

where $\epsilon_f(\theta) = s_0 \epsilon_0^{K} + c_0 \epsilon_0^{K'}$ and $\epsilon_e(\theta) = c_0 \epsilon_0^{K} + s_0 \epsilon_0^{K'}$. Diagonalization is therefore achieved for $\theta \equiv 0$ (mod $\pi$) or, if $s_0 c_0 \neq 0$, for

$$
\hat{\epsilon}_0^{K} - \hat{\epsilon}_0^{K'} = \mu_Z - u + \Omega_0 - \Omega_0 \lvert u \rvert = \mu_Z - \lambda_0 u \rightarrow 0,
$$

with $\lambda_0 = 1 - 2\Omega_0/u$. It is now clear that filled $0^0$ turns into filled $0^1$ across $u \sim u^{cr} = \mu_Z/\lambda_0$ via a global rotation of angle $\theta = \pi$.

Let us next note that $g^{11:K}_{\downarrow} \sim -1/2 c^2_0 |\theta|^2$ and $g^{11:K'}_{\downarrow} \sim -1/2 c_0 |\theta|^2$ barely differ for small $u \sim O(\mu_Z)$. The Coulomb interaction, acting within the $n = 1$ sector, thus remains almost invariant under global valley and spin rotations, and $\mathcal{H}^{\text{eff}}$ in Eq. (12) applies to the transition filled $1^K_{\downarrow} \rightarrow$ filled $1^L_{\downarrow}$ as well, with obvious replacement $G^{00} \rightarrow G^{11}$, $\hat{\epsilon}_0^{K'} \rightarrow \hat{\epsilon}_1^{K'}$, etc. The result is summarized in Eq. (57).

[1] K. S. Novoselov, E. McCann, S. V. Morozov, V. I. Fal’ko, M. I. Katsnelson, U. Zeitler, D. Jiang, F. Schedin, and A. K. Geim, Nat. Phys. 2, 177 (2006).
