Orbital Lamb shift and mixing of the pseudo-zero-mode Landau levels in ABC-stacked trilayer graphene

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In a magnetic field graphene trilayers support a characteristic multiplet of 12 zero(-energy)-mode Landau levels with a threefold degeneracy in Landau orbitals. It was earlier noted for bilayer graphene that Coulombic vacuum fluctuations, specific to graphene, lift the orbital degeneracy of such zero-energy modes and that these “Lamb-shifted” orbital modes, with filling, get mixed via the Coulomb interaction. It is pointed out that analogous orbital Lamb shift and mixing of zero-mode levels can also take place, with an enriched symmetry content, in ABC-stacked trilayer graphene; and its consequences are discussed in the light of experimental results.

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I. INTRODUCTION

Graphene,\(^1\)-\(^3\) an atomic layer of graphite that supports massless Dirac fermions, attracts great attention for its unique and promising electronic properties. Recently interest appears to center on bilayers and few layers of graphene, where the added layer degree of freedom makes the physics and applications of graphene richer. In particular, bilayer graphene and some types of multilayers enjoy the property that their band gaps are externally tunable.\(^4\)-\(^7\)

A notable signal of Dirac fermions is the fact that graphene, in a magnetic field, supports a characteristic set of zero-energy Landau levels, whose emergence and degeneracy have a topological origin in the chiral anomaly.\(^8\) Monolayer graphene has four such zero-energy levels owing to the spin and valley degeneracy, and they are responsible for the observed half-integer quantum Hall effect.\(^1\),\(^2\) In bilayer graphene there are eight such levels, with an extra twofold degeneracy\(^4\) in Landau orbitals \(n=0\) and \(1\). This “orbital” degeneracy is a consequence of topology and the added layer, and \(N\)-layer graphene necessarily has \(4N\) zero-energy Landau levels with \(N\)-fold orbital degeneracy. In the presence of Zeeman coupling, Coulomb interactions, etc., these zero-energy levels evolve into a variety of pseudo-zero-mode (PZM) levels, or broken-symmetry states, as discussed theoretically.\(^9\)-\(^11\) The interplay of orbital degeneracy and Coulomb interactions brings about a new realm of quantum phenomena\(^9\),\(^12\)-\(^16\) in the PZM sector, such as orbital mixing and orbital-pseudospin waves.

Graphene is distinguished from conventional electron systems by the feature that it is an intrinsically many-body system equipped with the quantum vacuum, or the valence band acting as the Dirac sea. Quantum fluctuations of the Dirac sea are sizable, even leading to ultraviolet divergences; and one encounters such field-theoretic (or many-body) phenomena as velocity renormalization,\(^17\) screening of charge,\(^18\) and nontrivial Coulombic corrections to cyclotron resonance.\(^19\)-\(^23\) Quantum fluctuations also affect the PZM levels substantially. They work to lift\(^24\) the orbital degeneracy of the PZM levels in bilayer graphene; each orbital mode responds to quantum fluctuations differently and gets shifted, just like the Lamb shift\(^25\) in the hydrogen atom, where the field-theoretic effect of quantum electrodynamics was revealed for the first time historically. The Lamb-shifted orbital modes get mixed via Coulomb interactions and govern the fine structure of the PZM sector.

A number of recent experiments\(^26\)-\(^32\) have verified that the electronic properties of graphene trilayers strongly depend on the stacking order, with Bernal (ABA)-stacked trilayers remaining metallic in contrast to rhombohedral (ABC-stacked) trilayers which exhibit a tunable band gap. Actually trilayers drew theorists’ attention\(^33\)-\(^36\) even before experiments and their rich electronic properties\(^37\)-\(^39\) have been under active study. Currently considerable attention\(^40\)-\(^42\) is directed to ABC-stacked trilayers which are a chiral generalization of bilayer graphene. In view of this, it is of interest to ask how the Coulombic vacuum and orbital dynamics generalizes to trilayers.

The purpose of this paper is to examine the effect of Coulombic vacuum fluctuations in trilayers and show that the orbital Lamb shift and orbital mixing of the PZM levels are also present, with an enriched symmetry content, in ABC-stacked trilayer graphene. It is noted, in particular, that level mixing takes place without level crossing; this mechanism would, for high-quality samples, lead to an observable sequence of fully-split broken-symmetry quantum Hall states in the PZM sector.

In Sec. II we briefly review some basic features of the PZM levels in ABC-trilayer graphene, and in Sec. III show that vacuum fluctuations lift their orbital degeneracy. In Sec. IV we discuss in a simplified setting how orbital mixing of the PZM levels takes place via the Coulomb interaction. In Sec. V we examine the hierarchy of broken-symmetry states under practical conditions. Section VI is devoted to a summary and discussion.
II. TRI_LAYER GRAPHENE

The ABC-stacked trilayer graphene consists of three graphene layers with vertically-arranged dimer bonds \((B_1, A_2)\) and \((B_2, A_3)\), where \((A_i, B_i)\) denote inequivalent lattice sites in the \(i\)-th layer. The interlayer coupling \(\gamma_0 \equiv \gamma_{B,A_i} \sim 3\) eV is related to the Fermi velocity \(v = (\sqrt{3}/2)u L_{70}/h \sim 10^6\) m/s in monolayer graphene. Interlayer hopping via the nearest-neighbor dimer coupling \(^{43}\gamma_1 \equiv \gamma_{A,B_i} = \gamma_{B,A_i} \sim 0.4\) eV leads to soft cubic spectra \(^{33} \propto \left| \mathbf{p} \right|^3\) in the low-energy branches \(|\epsilon| < \gamma_1\).

The effective Hamiltonian for ABC-stacked trilayer graphene with such intralayer and interlayer couplings is written as

\[
H_{\text{tri}} = \int d^2\mathbf{x} \left[ (\Psi^K)^\dagger \mathcal{H}_K \Psi^K + (\Psi^{K'})^\dagger \mathcal{H}_{K'} \Psi^{K'} \right],
\]

\[
\mathcal{H}_K = \begin{pmatrix} D_1 & V \n V^\dagger & D_2 \n W^\dagger & \n D_3 \end{pmatrix},
\]

\[
D_i = \begin{pmatrix} U_i \n v \n p \n \bar{p} \n U_i \end{pmatrix}, \quad V = \begin{pmatrix} -v_4 p^\dagger \n v_3 p \n \gamma_1 \n -v_4 p^\dagger \end{pmatrix},
\]

\[
W = \begin{pmatrix} 0 \n \gamma_2/2 \n 0 \n 0 \end{pmatrix},
\]

(1)

with \(p = p_x + ip_y\) and \(p^\dagger = p_x - ip_y\). Here \(\Psi^K = (\psi_{1A}, \psi_{1B}, \psi_{2A}, \psi_{2B}, \psi_{3A}, \psi_{3B})^\dagger\) stands for the electron field at the \(K\) valley. \(v_3\) and \(v_4\) are related to the non-leading interlayer couplings \(\gamma_3 \equiv \gamma_{A_1B_2}\) and \(\gamma_4 \equiv \gamma_{A_1A_2}\), respectively, and \(\gamma_2 \equiv \gamma_{A_1B_3}\). \((U_1, U_2, U_3)\) stand for the on-site energies of the three layers; we take \(U_2 = 0\) without loss of generality. As in bilayer graphene, \(^4\) these biases \((U_i)\) open a tunable band gap \(^{33} \sim U_1 - U_3\). \(\mathcal{H}_K\) is diagonal in (suppressed) electron spin.

The Hamiltonian \(\mathcal{H}_{K'}\) at another valley is given by \(\mathcal{H}_K\) with \(p \rightarrow -p_x + ip_y = -p^\dagger\) and \(p^\dagger \rightarrow -p\), and acts on a spinor of the same sublattice content as \(\Psi^K\). Actually, \(\mathcal{H}_{K'}\) is unitarily equivalent to \(\mathcal{H}_K\) with the sign of \(v_3\) and \(\gamma_2\) reversed and with layer 1 and layer 3 interchanged,

\[
S^\dagger \mathcal{H}_K S = \mathcal{H}_{K'}|_{-v_3, -\gamma_2, U_1 \leftrightarrow U_3},
\]

\[
S = \begin{pmatrix} \sigma_1 \n -\sigma_2 \n -\sigma_2 \n \sigma_2 \end{pmatrix}. \tag{2}
\]

In view of this, we adopt \(\mathcal{H}_{K'} = S^\dagger \mathcal{H}_K S\) for \(\mathcal{H}_{K'}\), and simply pass to the \(K'\) valley by reversing the sign of \(v_3\) and \(\gamma_2\) and interchanging \(U_1\) and \(U_3\) in the \(K\)-valley expressions. Nonzero \(v_3, \gamma_2\) and bias \(U_1 - U_3\) thus act as valley-symmetry breakings. Remember that in this representation \(\mathcal{H}_{K'}\) acts on a spinor of the form \(\Psi^{K'} = (\psi_{1A}, \psi_{1B}, \psi_{2A}, \psi_{2B}, \psi_{3A}, \psi_{3B})^\dagger\).

A direct link between the \(K\)- and \(K'\)-valley representations, such as Eq. (2), was also noted\(^{24}\) for bilayer graphene. We remark that such a link is not shared by \(ABA\)-stacked trilayers, where the Landau-level spectra significantly differ between the two valleys for nonzero biases (though they coincide for zero bias).

We have discussed the general structure of trilayer parameters for completeness. For our present analysis of quantum effects in \(ABC\) trilayers we retain only the leading parameters \((v, \gamma_1, U_i)\); the effect of nonleading couplings \((v_3, v_4, \gamma_2)\) is discussed later in Sec. V. In addition, we focus on the case of a symmetric bias \(^{33}\) by choosing \(U_3 = -U_1 = u/2\).

Let us place trilayer graphene in a strong uniform magnetic field \(B_z = B > 0\) normal to the sample plane; we set, in \(\mathcal{H}_{K'}, p \rightarrow \Pi = p + eA\) with \(A = A_x + i A_y = -B y\), and denote the The magnetic length as \(\ell = 1/\sqrt{eB}\); setting \(a \equiv \sqrt{2eB}/\Pi\) then yields \(|a, a|^2 = 1\). It is easily seen that the eigenmodes of \(\mathcal{H}_K\) have the structure

\[
\Psi_n = \begin{pmatrix} (n - 3) b_1^{(1)} \n |n - 2\rangle d_1^{(1)} \n |n - 2\rangle b_2^{(2)} \n (|n - 1\rangle d_2^{(2)} \n |n - 1\rangle b_3^{(3)} \n |n\rangle d_3^{(3)}) \end{pmatrix}^t \tag{3}
\]

with \(n = 0, 1, 2, \cdots\), where only the orbital eigenmodes are shown using the standard harmonic-oscillator basis \(|n\rangle\) (with the understanding that \(|n\rangle = 0\) for \(n < 0\)). The coefficients \(v_n = (b_1^{(1)}, d_1^{(1)}, b_2^{(2)}, d_2^{(2)}, b_3^{(3)}, d_3^{(3)})^t\) for each \(n = 3, 4, \ldots\) are given by the eigenvectors (chosen to form an orthonormal basis) of the reduced Hamiltonian \(\hat{H}_{\text{red}} \equiv \omega_c \hat{H}_n\) with

\[
\hat{H}_n = \begin{pmatrix} -M & \sqrt{n - 2} & 0 & \cdots & 0 \\
\sqrt{n - 2} & -M & \sqrt{n - 1} & \cdots & 0 \\
0 & \sqrt{n - 1} & -M & \cdots & \hat{\gamma} \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & \hat{\gamma} & M & \sqrt{n} \end{pmatrix},
\]

\[
\hat{\gamma} = \sqrt{\omega_c/\ell} = 36.3 \times v/10^6 \text{ m/s} \sqrt{B/|\Pi|} \text{ meV}, \tag{4}
\]

with \(v\) in units of \(10^6\) m/s and \(B\) in tesla, is the characteristic cyclotron energy for monolayer graphene; \(M \equiv \frac{1}{2} u/\omega_c\) and \(\hat{\gamma} \equiv \gamma_1/\omega_c\). Note that eigenvectors \(v_n\) can be taken real since \(\hat{H}_n\) is a real symmetric matrix.

Solving the secular equation shows that there are 6 branches of Landau levels for each integer \(n \geq 3\). We denote the eigenvalues as \(\epsilon_{-n'} < \epsilon_{-n''} < \epsilon_{-n} < \epsilon_{n''} < \epsilon_{n'} < \epsilon_{n}\), so that the index \(n')\) reflects the sign of \(\epsilon_n\); \(|\epsilon_{-n'}| > |\epsilon_1|\) and \(|\epsilon_{n''}| > |\epsilon_1|\). The \(|n| = 3\) levels, e.g., consist of the \(n = (-3, -3', -3'')\) branches.

There are also solutions for \(n = 2, 1\) and 0, for which \(\hat{H}_n\) is reduced to a matrix of smaller rank 5, 3 and 1. For \(n = 0\), \(\hat{H}_{\text{red}}\) has an obvious eigenvalue \(\epsilon_0 = U_3 = u/2\) with eigenvector \(v_0 = (0, 0, 0, 0, 0, 1)^t\) or

\[
\Psi_0 = (0, 0, 0, 0, 0, 0)^t. \tag{6}
\]

For \(n = 1\), \(\hat{H}_{\text{red}}\) has three eigenvalues \(\epsilon_1, \epsilon_{\pm 1'}\), which, for \(u = 0\), read \((0, \pm \sqrt{\gamma + 1})\omega_c\). The zero-energy solution, in particular, takes the form:

\[
\Psi_1^{u=0} = (c_1, 0, 0, 0, -\kappa |0), 0, (1)|^t, \tag{7}
\]
with \( \kappa \equiv 1/\hat{\gamma} \) and \( c_1 = \hat{\gamma}/\sqrt{\hat{\gamma}^2 + 1} = 1/\sqrt{1 + \kappa^2} \). For
\( n = 2 \), \( \hat{\gamma}_{\text{rec}} \) has five eigenvalues \( (c_2, c_2, e_{\pm 2}^\ast, e_{\pm 2}^\ast) \), with
\( c_2 = 0 \) and \( |e_{\pm 2}^\ast| \sim |e_{\pm 2}^\ast| \sim \gamma_1 \) for \( u = 0 \). The zero-energy
solution takes the form
\[
\Psi_2 \equiv c_2 \left( 0, \sqrt{2} \kappa^2 |0, 0, -\sqrt{2} \kappa |1, 0, |2 \right)^t, \tag{8}
\]
with \( c_2 = \hat{\gamma}^2/\sqrt{2 + \hat{\gamma}^2 + \hat{\gamma}^2} = 1/\sqrt{1 + 2 \kappa^2 + 2 \kappa^2} \). Note that these zero-energy solutions \( (\Psi_0, \Psi_1, \Psi_2) \) reside predominantly on the \( B_2 \) lattice sites of the third layer; correspondingly, the zero-energy solutions at the \( K' \) valley reside predominantly on the \( A_1 \) sites of the first layer.

Of our particular concern are these three zero-energy modes \( (\Psi_0, \Psi_1, \Psi_2) \). For \( u = 0 \) there are 12 such zero-energy Landau levels differing in spin, valley and orbital \([n = (0, 1, 2)]\) degrees of freedom; their presence is dictated by the nonzero index of the Dirac Hamiltonian \( \mathcal{H}_{K} \oplus \mathcal{H}_{K'} \) with only \( v \) and \( \gamma_1 \) retained.

For nonzero bias \( u \neq 0 \) they evolve into the pseudo-zero modes with nonzero energies,
\[
(e_{1n}, e_{2n}, e_{3n}) = (1, 1 - z_1, 1 - z_2) u/2, \]
\[
z_1 = \kappa^2(c_1^2 + O(\kappa^6)), \]
\[
z_2 = 2\kappa^2(1 + 2\kappa^2)(c_2^2) + O(\kappa^6), \tag{9}
\]
where \( \hat{u} \equiv u/\omega_c \). One can also write \( e_{1n}^u \approx (c_1^2) u/2 \) and \( e_{2n}^u \approx (1 - 2\kappa^2)(c_2^2) u/2. \)

For a numerical estimation let us take, as typical values, \( \gamma_0 = 3.16 \text{ eV} \) (or \( u \approx 1.0 \times 10^9 \text{ m/s} \)) and \( \gamma_1 = 0.4 \) eV. They yield \( \hat{\gamma} \approx 3.41 \) and \( \kappa \approx 0.293 \) at \( B = 10 \text{ T} \), which in turn lead to \( c_1 \approx 0.960, c_2 \approx 0.918, z_1 \approx 0.08 \) and \( z_2 \approx 0.17 \). One thus has
\[
(e_{1n}^u, e_{2n}^u, e_{3n}^u) \approx (1, 0.92, 0.83) u/2 \tag{10}
\]
for \( u < \omega_c \).

One can pass to the \( K' \) valley by setting \( u \rightarrow -u \) in the \( K \) valley expressions. The eigensystems \( (e_{\alpha n}, v_{n \alpha}) \) at the two valleys are related as
\[
e_{\alpha n|K'} = -e_{-\alpha n|K}, \]
\[
b_{\alpha n|K'} = -b_{\alpha n|K}, d_{\alpha n|K'} = d_{\alpha n|K} \tag{11}
\]
for each mode \((n, n', n'')\) and \( i \in (1, 2, 3) \). For later convenience, we continue to use \( n = (0, 1, 2) \) to specify the PZM levels at the \( K' \) valley; one can thus effectively set \( n = \pm 0 \rightarrow 0, \pm 1 \rightarrow 1 \) and \( \pm 2 \rightarrow 2 \). When the interlayer bias \( u \) is turned on, these PZM levels go up or down oppositely at the two valleys, opening a band gap \( u \).

The Landau-level structure is made explicit by passing to the \([n, y_0]\) basis (with \( y_0 \equiv \ell^2 p_x \)) via the expansion \( \Psi^K(x) = \sum_n y_0 (x|n, y_0) \psi_{n \alpha}(y_0) \), where \( n \) refers to the level index, \( \alpha \in (\uparrow, \downarrow) \) to the spin, and \( a \in (K, K') \) to the valley. The charge density \( \rho_{-\mathbf{p}} = \int d^2x e^{i\mathbf{p}\cdot\mathbf{x}} \rho \) with \( \rho = (\Psi^K)\imath \Psi^K + (\Psi^{K'})\imath \Psi^{K'} \) is thereby written as
\[
\rho_{-\mathbf{p}} = \gamma_{\mathbf{p}} \sum_{k, n = -\infty}^{\infty} \sum_{\alpha, \alpha} g_{kn;\alpha \alpha} R_{\alpha \alpha;\mathbf{p}}, \tag{12}
\]
where \( \gamma_{\mathbf{p}} \equiv e^{-e^2 p_x/4}; \mathbf{r} = (i\ell^2 \partial/\partial y_0, y_0) \) stands for the center coordinate with uncertainty \([x_\alpha, y_\alpha] = i\ell^2 \); the level sum \( \sum_n \) is taken over possible \((n, n', n'')\).

The coefficient matrix \( g_{kn;\alpha \alpha} = g_{kn;\alpha \alpha} \) at valley \( a \in (K, K') \) is constructed from the eigenvectors \( v_{n \alpha} \).
\[
g^{kn}_{\mathbf{p}} = b_{(k')_{\alpha \alpha \alpha}} f^{(k')_{\alpha \alpha \alpha}} f_{(k)_{\alpha \alpha \alpha}} \tag{13}
\]
for \( n \geq 0 \), and \( f_{kn}^{(k)} \equiv (f_{kn})_{(k)_{\alpha \alpha \alpha}} \); \( \bar{q} = y \ell (x - y p_y) \); it is understood that \( f_{kn}^{(k)} = 0 \) for \( k < 0 \) or \( n < 0 \). As seen from Eq. (11), \( g_{kn;\alpha \alpha} \) at the two valleys are related as
\[
g_{m n}^{kn}_{\mathbf{p}} = g_{m, n - |K', k'' |\alpha \alpha} = g_{m, n - \alpha \alpha, 2, 3, 1} \tag{15}
\]

Within the \( n \in (0, 1, 2) \) sector, \( g_{kn;\alpha \alpha} \) are functions of \((u^2, \kappa^2)\) and are thus common to both valleys; for \( u = 0 \), they read
\[
g_{00}^{m n} = 1, g_{01}^{m n} = c_1 \ell p_x /\sqrt{2}, g_{10}^{0 n} = -c_1 \ell p_y /\sqrt{2}, \]
\[
g_{02}^{0 n} = c_2 \ell^2 p_x /2(\sqrt{2}), \]
\[
g_{11}^{m n} = 1 - (c_1)_{\alpha \beta \alpha}^2 \ell^2 p_x^2, g_{12}^{m n} = \lambda_p g_{01}^{m n}, \]
\[
g_{22}^{m n} = 1 - (c_2)_{\alpha \beta \alpha}^2 (1 + \kappa^2) \ell^2 p_x^2 - \frac{1}{2} \lambda_p (\ell^2 p_y^2)^2, \]
\[
\lambda_p = \sqrt{2}(1 + \kappa^2 - \frac{1}{4} \ell^2 p_x^2) \tag{16}
\]
with \( c_1 = 1/\sqrt{1 + \kappa^2} \) and \( c_2 = 1/\sqrt{1 + 2 \kappa^2 + 2 \kappa^2} \).

From now we frequently suppress summations over levels \( n \), spins \( \alpha \) and valleys \( a \), with the convention that the sum is taken over repeated indices. The Hamiltonian \( H^{\beta \alpha} \) projected to the PZM levels is thereby written as
\[
H_{\alpha \beta} = e_{\alpha} \delta R_{\beta \beta}^{mn} - \mu_\beta (T_3)_{\beta \alpha} R_{\alpha \alpha}^{mn;\alpha \alpha} \tag{17}
\]
with \( n \in (0, 1, 2) \) and \( \delta R_{\alpha \beta}^{mn;\alpha \alpha} = F_{mn;KK'} - R_{mn;KK'}^{mn;\alpha \alpha} \).

Here the Zeeman term \( \mu_\beta = g_{\beta} \mu_B B / 0.12 B[T] \text{ meV} \) is introduced via the spin matrix \( T_3 = \sigma_3/2 \).

### III. VACUUM FLUCTUATIONS

In this section we examine the effect of Coulombic quantum fluctuations on the PZM multiplet. The Coulomb interaction is written as
\[
V = \frac{1}{2} \sum_{\mathbf{p}} \rho_{-\mathbf{p}} \rho_{-\mathbf{p}}. \tag{18}
\]
where \( v_p = 2\pi a/(|e_b| |p|) \) with \( a = e^2/(4\pi \epsilon_0) \approx 1/137 \) and the substrate dielectric constant \( \epsilon_s \). \( \sum_p = \int d^2 p/(2\pi)^2 \). For simplicity we ignore the difference between the intralayer and interlayer Coulomb potentials.

In this paper we generally focus on many-body ground states \( |G\rangle \) with a homogeneous density, realized at integer filling factor \( \nu \in [-6, 6] \). We set the expectation values \( \langle G | R_{\alpha\beta} | k \rangle = \delta_{\alpha \beta} \rho_0 \nu_{\alpha\beta} \) with \( \rho_0 = 1/(2\pi \ell^2) \) and \( \delta_{\alpha \beta} = (2\pi)^2 \delta^2(\mathbf{k}) \); accordingly, the filling factor \( \nu_{\alpha\alpha} = 1 \) for a filled level specified by \( (n, a, \alpha) \).

Let us define the Dirac sea \( |DS\rangle \) as the valence band with levels below the PZM sector (i.e., levels with \( n \leq -3 \)). The bilayer case.

In this section we examine how the PZM sector changes as the interlayer Coulomb potential increases. Fortunately one can isolate the divergence and even evaluate \( V_{\text{dirac}}^{\text{DS}} \) for zero bias \( u \to 0 \), as done for the bilayer case.\(^{24}\) Note first that, as seen from Eq. (15),

\[
\gamma_{mn}^{m'n'} |K = g_{mn}^{m'n'} |k' = g_{mn}^{m'n} \quad \text{for} \quad u = 0,
\]

we use the completeness relation\(^{24}\)

\[
\sum_{n=-\infty}^{\infty} |g_{mn}^n|^2 = \epsilon_k^2 \ell^2/2
\]

to extend the sum over \( n \) to its complement \( \sum_{n \in \text{DS}} \) as well. The result is

\[
\sum_{n \in \text{DS}} |g_{pn}^n|^2 = \frac{1}{2} \left( \epsilon_k^2 \ell^2/2 - |g_{j0}^0|^2 - |g_{j1}^1|^2 - |g_{j2}^2|^2 \right),
\]

for \( j = (0, 1, 2) \). Equation (21) was noted earlier with a formal proof; a direct proof of it is given in Appendix A. The \( \epsilon_k^2 \ell^2/2 \) term in Eq. (22), though leading to a divergence upon integration over \( p \), is common to all levels \( j \) and is safely omitted. We thus take the rest as the regularized expression for \( \sum_{n \in \text{DS}} |g_{pn}^n|^2 \).

The regularized Dirac-sea contribution thus reads

\[
V_X^{\text{DS}} u \to 0 \to j \epsilon_0 R_{\alpha a, 0}^{00\alpha a} + \epsilon_1 R_{\alpha a, 0}^{11\alpha a} + \epsilon_2 R_{\alpha a, 0}^{22\alpha a},
\]

IV. MIXING OF THE PZM LEVELS

In this section we examine how the PZM sector changes in spectrum with filling. The first step is to extract from \( V_X \) in Eq. (19) the exchange interaction acting within the \( n = (0, 1, 2) \) sector,

\[
V_X^{pZ} = - \sum_p v_p \gamma_{p}^2 \Gamma_p^{mn} R_{0}^{mn},
\]

\[
\Gamma_p^{00} = \nu_{0}^{0} |g_p^{00}|^2, \quad \Gamma_p^{11} = \nu_{0}^{11} |g_p^{11}|^2, \quad \Gamma_p^{22} = \nu_{0}^{22} |g_p^{22}|^2,
\]

\[
\Gamma_p^{0} = g_p^{0} |g_p^{0}|^2, \quad \Gamma_p^{1} = g_p^{0} g_p^{01} \nu_{10} + g_p^{0} g_p^{02} \nu_{21},
\]

\[
\Gamma_p^{2} = g_p^{0} g_p^{02} \nu_{02} + g_p^{0} g_p^{02} \nu_{22}, \quad \Gamma_p^{20} = g_p^{0} g_p^{02} \nu_{02},
\]

Integration over \( p \), with the aid of the formula

\[
\sum_p v_p \gamma_{p}^2 [1, q, q^2, q^4, q^6, q^8] = [1, 1, 1, 3, 15, 105] \tilde{V}_c
\]

with \( q = \ell |p| \), then yields

\[
\tilde{V}_c = \frac{1}{4} \left[ 1 + c_2^2 (\frac{15}{16} + \frac{5}{16}) \right] \tilde{V}_c,
\]

where \( c_2^2 \equiv (c_1)^2 \).\(^{23}\) Numerically,

\[
(c_0^2, \epsilon_0, c_2^2) = (0.888, 0.777, 0.641) \tilde{V}_c
\]

for \( \gamma = 1/\epsilon \approx 3.41 \) at \( B = 10 \) T.

Vacuum fluctuations thus shift the \( n = 0, 1, 2 \) modes differently and the splitting among \( (\epsilon_0^2, \epsilon_1^2, c_2^2) \) reflects the difference in their spatial distributions, as is clear from Eq. (24). The empty PZM levels are ordered as \( c_0^2 < c_1^2 < c_2^2 > 0 \). Actually the spectra vary with filling of the PZM sector. Note Eq. (20), which tells us to include extra contributions \( -|g_{mn}^n|^2 \) for \( \epsilon_j^2 \), when the \( n = (0, 1, 2) \) level is filled. In particular, when the PZM sector is filled up, one finds that \( \{\epsilon_j^2\} \) change sign so that they are ordered as \( c_0 < \epsilon_1 < c_2 < 0 \).

Let us next suppose filling the lowest-lying \( n = 2 \) level first in the empty PZM sector (for \( u = \mu_Z = 0 \)). One then finds \( \epsilon_2^2 \approx 0.054 \tilde{V}_c \) for \( g \approx 3.41 \). If, instead, the highest-lying \( n = 0 \) level were first filled, one would find \( \epsilon_0^2 \approx -0.11 \tilde{V}_c \) here as well. This puzzling situation suggests that one cannot reach the true ground state by filling the \( n = 2 \) level alone. It is clear now that one has to diagonalize the exchange interaction (19), with mixing among the \( n = (0, 1, 2) \) orbital modes taken into account.
where \( m, n \in (0, 1, 2); \Gamma_{p}^{0} \equiv (\Gamma_{p}^{0})^*, \Gamma_{p}^{2} \equiv (\Gamma_{p}^{2})^*, \) etc. For conciseness, the spin and valley indices have been suppressed in the above; \( \nu_{mn} R_{0}^{0} \equiv \rho_{a b c}, \frac{\partial}{\partial \phi_{a b c}} \) one reads \( \nu_{mn} R_{0}^{0} \equiv \rho_{a b c} \).

Let us, for the moment, freeze the spin and valley degrees of freedom and focus on the orbital degrees of freedom. The PZM sector then consists of three levels \( n \in (0, 1, 2) \) governed by the effective Hamiltonian \( \mathcal{V} = V_{D} + V_{X} = H^{mn} f R_{0}^{0} + H^{mn} \equiv \epsilon_{n}^{0} f^{mn} - \sum_{p}^{2} \frac{\partial}{\partial \phi_{a b c}} \phi_{a b c}. \) Note that \( \Gamma_{p}^{0} \) are real for real filling factors \( \nu_{mn} \), which we take. It therefore suffices to use a real \( O(3) \) rotation, rather than a full \( SU(3) \) rotation, to diagonalize the \( 3 \times 3 \) real symmetric matrix \( H^{mn} \). We thus rotate \( \psi^{m} = (\psi^{0}, \psi^{1}, \psi^{2}) \) in orbital space,

\[
\psi_{m}(\theta) = [\mathcal{U}(\theta_{2}, \theta_{1}, 0)]^{mn} \Phi^{m}(\theta),
\]

with three Euler angles \( (\theta_{2}, \theta_{1}, 0) \) parameterizing

\[
\mathcal{U}(\theta_{2}, \theta_{1}, 0) = e^{i\theta_{2} \varepsilon_{2} e^{i\theta_{1} \varepsilon_{1}}} e^{i\theta_{0} \varepsilon_{0}},
\]

where the spin-1 generators \( (\varepsilon_{a b c})^{\pm} \equiv i e^{a b c} \) in terms of the totally antisymmetric tensor \( e^{a b c} \) with \( e^{012} = 1 \). Note that \( \theta_{0} \) mixes \( n = (1, 2), \theta_{1} \) mixes \( (0, 2) \), etc.

Via the rotation, \( \mathcal{V} = H^{mn} f R_{0}^{0} = \mathcal{H}^{mn} f R_{0}^{0} + \mathcal{H} = \mathcal{U}^{+} \mathcal{H} \mathcal{U}, \) where \( R_{0}^{0}, \mathcal{H}^{mn} \) stand for the charge operators for \( \Phi^{m} \), i.e., \( \mathcal{H}^{mn} f \) with \( \mathcal{H}^{mn} \rightarrow \mathcal{H}_{mn}^{n b} \). The transformed fields \( \Phi^{n} \) are taken to diagonalize \( \mathcal{H}^{mn} f \) and hence the associated filling factors as well, \( \nu_{n} \propto (G(\Phi^{m}) \mathcal{H}^{mn} f G(0)) \) with \( 0 \leq \nu_{n} \leq 1 \) and \( n \in (0, 1, 2) \); one can now write

\[
\nu_{mn} = \langle U_{mn} \rangle \nu_{n} \langle \mathcal{U}^{\dagger} \rangle_{n}.\]

Let us start filling the empty PZM sector at (relative) filling factor \( n_{l} = 0 \). Obviously, in view of level splitting (28), it is the lowest-lying \( n = 2 \) level (\( \Phi^{2} \)) that starts to be filled. To follow how it evolves let us suppose that it is filled with fraction \( n_{l} \leq 1 \) and substitute \( (N_{0}, N_{1}, N_{2}) = (0, n_{l}, 0) \). \( \mathcal{H}^{mn} f \) is diagonalized if one can adjust \( (\theta_{0,1}), \theta_{2}, \theta_{0,1} \) so that \( \mathcal{H}^{01} = \mathcal{H}^{22} = \mathcal{H}^{12} = 0 \).

Note first that, with no level mixing, i.e., \( \theta_{0} = \theta_{1} = \theta_{2} = 0 \), the eigenvalues \( \{\mathcal{H}^{mn} f \} \) simply go down with increasing \( n_{l} \). Note next that, to first order in \( \{\theta_{n}\} \),

\[
\mathcal{H}^{12} \approx (0.136 - 0.268 n_{l}) \theta_{0} + ...,
\]

\[
\mathcal{H}^{02} \approx -0.247 - 0.130 n_{l} \theta_{1} + ...
\]

\[
\mathcal{H}^{01} \approx -0.201 n_{l} \theta_{0} + (0.111 + 0.0626 n_{l}) \theta_{2} + ...\]

This structure reveals that \( \theta_{0} = \theta_{1} = \theta_{2} = 0 \) for \( n_{l} < n_{c} \approx 0.507 \) while \( \theta_{0} \neq 0 \) is possible for \( n_{l} > n_{c} \). Solving for \( \{\theta_{n}\} \) numerically for \( n_{l} \geq n_{c} \), shows that the energy eigenvalue \( \mathcal{H}^{22} f \) is indeed lowered for \( n_{l} > n_{c} \) with \( \theta_{0} \neq 0 \). One can then reach the \( n_{l} = 1 \) state, and setting \( (N_{0}, N_{1}, N_{2}) \rightarrow (0, n_{l} - 1, 1), \) etc., takes one further to the \( n_{l} = 2 \) and 3 states.

Figure 1 (a) shows how angles \( \{\theta_{n}\} \) vary as \( n_{l} \) is increased from 0 to 3. Actually we find another solution which differs from one shown in the figure by signs, \( (\theta_{2}, \theta_{1}, 0) \rightarrow (-\theta_{2}, \theta_{1}, -\theta_{0}) \). These two solutions are related by a unitary transformation \( \mathcal{Y} = \text{diag} (x, -1, 1) \), with \( \mathcal{U}^{-1} \mathcal{Y} \mathcal{U} \mathcal{Y}^{-1} \) yielding the relevant portion of \( \mathcal{H}_{A} \) as written.

\[
\epsilon_{\text{exp}} n_{l} = 0.53 \mathcal{V}_{c},
\]

considerably smaller than the full Coulombic gap \( \epsilon_{c} = 1.28 \mathcal{V}_{c} \).

A special feature associated with orbital mixing is that charge carriers acquire electric dipole moment, as noted earlier\(^{12,14} \) for bilayer graphene. To see this let us consider coupling to an external scalar potential \( A_{0} \), with the Hamiltonian \( \mathcal{H} = -e \sum_{p} (A_{0})_{p} \rho_{p} \). Note that \( \gamma_{p}^{01}, \gamma_{p}^{12} \) in \( \rho_{p} \) \( \propto \mathcal{V} \), which implies that orbital mixing gives rise to coupling to an inplane electric field \( E_{||} = (E_{x}, E_{y}) = -\nabla A_{0} \). Indeed, for a spatially almost uniform field \( E_{||} \), the relevant portion of \( \mathcal{H}_{A} \) is written as

\[
\mathcal{H} = e_{\text{exp}}/n_{l} = 0.53 \mathcal{V}_{c},
\]

or 1.28 \( \mathcal{V}_{c} \).
\[ H_A \approx h_A^{mn} R_0^{mn} \text{ with } h_A = -c_2 (\ell / \sqrt{2}) (E_y T_y + E_x T_x), \]

where

\[ T_y = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad T_x = \frac{1}{\lambda} \begin{pmatrix} 1 & -1 \\ 1 & -\lambda \end{pmatrix} \]

act on fields \((\psi^0, \psi^1, \psi^2)\) and \(\lambda \equiv \lambda_{p=0} = \sqrt{2} (1 + \kappa^2) c_2\).

The expectation value \(\langle G | H_A | G \rangle\) then reads

\[ \langle G | H_A | G \rangle \approx \rho_0 \int d^2 \mathbf{x} \left( -\mathbf{d} \cdot \mathbf{E}_\parallel \right), \]

where \(\mathbf{d} = (0, d_y)\) and \(d_y = (\ell / \sqrt{2}) c_1 D(\eta_{\mu})\) with function \(D(\eta_{\mu}) \equiv (T_y + \lambda T_x)^{mn} V^{mn}\) given by the plot in Fig 1 (c). This shows that electrons acquire electric dipole moment of magnitude \(|d_x| = (\ell / \sqrt{2}) c_1 |D(\eta_{\mu})|\) (per particle), pointing in the \(y\) axis for the present choice of wave functions.

Actually the electric dipole can point in any direction (in general, perpendicular to traveling waves) at no cost of energy. To see this let us consider a phase rotation of the form (within \(SU(3)\) rotations), \(\psi^a \rightarrow \psi'^a\) with \(\psi^0, \psi^1, \psi^2 = (e^{-i\phi} \psi^0, e^{i\phi} \psi^1, e^{i\phi} \psi^2)\). Note that \(g^{kn}_{\mu}\) are thereby transformed so that \(\rho_{\mathbf{p}}\) remains invariant. This transformation leaves \(\mathcal{V} = V_X^{\text{DS}} + V_X^{\text{PS}}\) invariant; hence, the spectrum remains unchanged. Still the electric dipole thereby rotates so that

\[ \mathbf{d} \equiv (d_x, d_y) = (\sin \phi, \cos \phi) \left| \mathbf{d}_x \right|. \]

It is now clear that a pair of solutions \(\psi\) and \(Y \psi\), encountered earlier, differ by a rotation by \(\pi\) of coordinates in the sample plane.

V. GENERALIZATION

In this section we recover the electron spin and valley degrees of freedom and explore the PZM sector with both \(\mu_Z\) and bias \(u\), using the full Hamiltonian

\[ H_{\text{eff}} = H_u + V_X^{\text{DS}} + V_X^{\text{PS}}. \]

We leave \(u\) arbitrary but keep \(|u| \ll V_c\) so that one can still use the \(u = 0\) expressions for \(\mathcal{V} = V_X^{\text{DS}} + V_X^{\text{PS}}\), with \(u\) retained only in \(H_u\) as a small perturbation.44

In addition, we ignore the difference between the intra- and interlayer Coulomb potentials that leads to a valley-symmetry breaking of \(O(V_c, d / \ell)\), with the layer separation \(d \sim 0.35 \text{ nm} \ll \ell\). This breaking contains capacitance energies that determine how valleys rotate. In conventional bilayer systems, the capacitance energy, though as tiny as \(O(V_c, d^2 / \ell^2)\), is positive and induces a valley rotation \((K, K') \rightarrow K \pm K'\), which makes the symmetric states \(\propto K + K'\) lower in energy. In contrast, for bilayer graphene, capacitance energies turn out to be negative and suppress possible valley rotations for \(u \sim 0\).

Experimentally, it is difficult to directly observe valley quantum numbers, especially from the sequence in which the broken-symmetry states emerge with varying filling factor \(\nu\) or magnetic field \(B\). The sequence is governed by the Coulombic gaps, which, though possibly triggered by small valley or spin or orbital breaking, are practically insensitive in magnitude to small \(|u| \ll V_c\). (In contrast, for large bias \(u\), the valley is naturally polarized in either \(K\) or \(K'\), depending on the sign of \(u\).) For this reason, instead of a (rather laborious) analysis of capacitance energies, we here simply suppose a possible valley rotation \((K, K') \rightarrow (+, -)\) without specifying its details for small \(u\); we take the (-) state to be lower in energy for each \(n \in \{0, 1, 2\}\) and spin \(\alpha \in \{\uparrow, \downarrow\}\).

In \(H_{\text{eff}}\) the exchange interaction \(V_X^{\text{DS}} + V_X^{\text{PS}}\) conserves both valley and spin, but breaks the orbital degeneracy. In contrast, the small perturbation \(H_u\) lifts all three degeneracies. Figure 2 depicts the empty PZM sector (at \(\nu = -6\)) governed by \(H_u + V_X^{\text{PS}}\), with level spectra

\[ \epsilon_n^{\uparrow \downarrow} = \epsilon_n^{\uparrow} \pm \epsilon_n^{\downarrow} - \frac{1}{2} \mu_Z, \quad \epsilon_n^{\pm \uparrow} = \epsilon_n^{\pm} + \epsilon_n^{\mp} + \frac{1}{2} \mu_Z, \]

in obvious notation. There are two possible level patterns, depending on (i) \(0 \leq u < u_{\text{cr}}\) (of spinbreaking domination) or (ii) \(u > u_{\text{cr}}\) (of valley-breaking domination) with \(u_{\text{cr}} \equiv \mu_Z/(1 - z_2) \approx 1.2 \mu_Z\) at \(10T\). In Eq. (38), for definiteness, we have assumed no valley rotation and \(u \geq 0\), so that \((+, -, -) = (K, K')\). When a valley rotation is induced (for small \(u\)), the \(\pm \epsilon_n^{\alpha}\) portions are replaced by more complex expressions, which, at any rate, are small for small \(u\), and the level pattern (i) in Fig. 2 remains essentially intact. (For consistency, we set \(u \rightarrow 0\) in our discussion for case (i) below.)

Let us start filling the empty PZM sector. Obviously, with \(|u|, \mu_Z \ll V_c\), the orbital splitting among \(\{\epsilon_n^{\alpha}\}\) singles out the \(2-\uparrow\) level as the lowest-lying one in both cases (i) and (ii). It is thus the \(2-\uparrow\) level that is filled first. As it is being filled, it comes down in energy, followed by the \(0-\uparrow\) and \(1-\uparrow\) levels coupled via the exchange interaction \(V_X^{\text{PS}}\). These three levels undergo orbital mixing, discussed in the previous section, through the \(\nu = -5\) and -4 states until one reaches the \(\nu = -3\) state, which is orbitaly neutral (an \(SU(3)\) singlet) but is polarized in valley and spin \((-\uparrow, +\uparrow\)). The associated \(\nu = -3\) level gap is a valley gap for case (i) and a spin gap for case (ii),

\[ \epsilon_{\nu = -3}^{\text{gap}}(\alpha) = 2 \epsilon_2^{\nu} + \mu_Z. \]
with $2\epsilon_2^\nu \approx 1.28\tilde{V}_c$. Similarly, as one goes up from $\nu = -3$ to $\nu = 0$, essentially the same orbital mixing is repeated for the ($+\uparrow$) sector in case (i) and for the ($-\downarrow$) sector in case (ii); analogously for the $\nu \in \{0, 6\}$ domain.

Figures 3 (a) and 3 (b) show the resulting spectra of the PZM multiplet at each integer filling factor $\nu \in [-6, 6]$. They differ in pattern for (i) $u \sim 0$ and (ii) $u > u_{cr}$, but form a perfectly particle-hole symmetric spectrum for the PZM sector in each case. The $\nu = \pm 2, \pm 1$ and 0 states thus differ in composition, depending on $u$. The $\nu = 0$ state, in particular, is spin-polarized for $u \sim 0$ and valley-polarized for $u > u_{cr}$, with a gap

$$e_{\nu=0}(\nu) \approx 2\epsilon_2^\nu + \mu_Z,$$

$$e_{\nu=0}(\nu) \approx 2\epsilon_2^\nu + (1 - z_2)u - \mu_Z. \quad (40)$$

As to the $\nu = -5$ gap, especially for case (ii) (of relatively large $u$), we note the following: $(\epsilon_0^\nu, \epsilon_1^\nu, \epsilon_2^\nu)$ in $H_u$, via the rotation $U$, turns into $(0.96, 0.899, 0.897)u/2$, i.e., $\epsilon_1^\nu \approx \epsilon_2^\nu$ at $\nu = -5$; similarly, $\epsilon_0^\nu \approx \epsilon_1^\nu$ at $\nu = -4$. This suggests that the $\nu = (\pm5, \pm4, \pm3, \pm2, \pm1)$ gaps are practically insensitive to both bias $u$ and $\mu_Z$, and equal to $e_{\nu=0}(\nu) \approx 0.53\tilde{V}_c$. \quad (41)

These orbital gaps are considerably smaller than the (Coulomb-enhanced $\nu = 0, \pm 3$) spin or valley gaps,

$$e_{\nu=\pm1, \pm2, \pm3} < e_{\nu=\pm1, \pm2, \pm3} \lesssim e_{\nu=0} \approx 0, \quad (42)$$

in conformity with Hund’s rule.\cite{9, 40} These $\nu = \pm 1, \pm 2, \ldots$ orbital gaps and the $\nu = \pm 3$ valley gaps for $u \sim 0$ barely depend on $\mu_Z$ and will therefore be insensitive to an additional parallel field $B_\parallel$ in experiments with a tilted magnetic field, in contrast to the $\nu = 0$ spin gap for $u \sim 0$. For bilayer graphene, the corresponding gaps take place at $\nu = -3$ and -2, and it was observed\cite{46} that the associated resistance minima are barely affected by $B_\parallel$.

The orbitally polarized states at $\nu = \pm 1, \pm 2, \pm 4, \pm 5$ have spontaneous electric dipole moment and may potentially be unstable\cite{12, 41, 42} against charge inhomogeneities. Their spectra may be modified (in random patterns or regular\cite{41, 42} patterns) around local charge concentrations but, as long as the orbital gaps survive, the quantum Hall states would emerge. Such an instability disappears when bias $u$ is sufficiently large to stabilize the valley-polarized states. For bilayer graphene full splitting of the PZM levels has indeed been observed.\cite{46, 47}

The transport properties of trilayers have been studied in a number of experiments.\cite{26, 31, 32} Experimentally there is clear evidence for formation of the quantum Hall states in the basic filling-factor sequence $\nu = \pm 4(N + 3/2) = \pm 6, \pm 10, \pm 14, \ldots$ for both $ABC$ and $ABA$-stacked trilayers. Evidence is yet very limited for the fine structure of the PZM sector with $|\nu| < 6$ in $ABC$ trilayers: An experiment,\cite{31} using a Hall-bar device, observed a weak anomaly in $\sigma_{xy}$ indicative of the developing $\nu = \pm 3$ gap. A clear signal for the $\nu = 0$ gap comes from the observation\cite{26, 30} of the insulating state at the Dirac point ($\nu = 0$) in $ABC$-trilayer devices, both suspended and substrate-supported ones, with the resistance rising exponentially with increasing $B$ and lowering temperature $T$. Experimentally, it is normally the $\nu = 0$ insulating state that is first observed as a nontrivial feature within the PZM sec-
tor of few-layer graphene. This suggests that the $\nu = 0$ gap is an interaction-enhanced gap rather than the far smaller intrinsic spin or valley gap. The $\nu = \pm 3$ gaps will be the next to be visible via quantized conductance. In view of Eqs. (39) and (40), the $\nu = 0$ gap will become even more prominent with increasing bias $u$, in contrast to the $\nu = \pm 3$ gaps.

Finally we wish to discuss possible effects of nonleading interlayer couplings $(v_4, v_3, \gamma_2)$. The effect of $v_4$ can be included in $\mathcal{H}_n$ of Eq. (4) while $v_3$ and $\gamma_2$ induce transitions that go outside the PZM sector, as seen from the solutions in Eqs. (6) - (8). Accordingly the spectra $(\epsilon_0, \epsilon_1, \epsilon_2)$ are corrected to first order in $v_4/u$ and to second order in $v_3/v$ and $\gamma_2/\gamma_0$. With typical values $v_4/v \equiv r_4 \sim 0.01$, $v_3/v = \gamma_3/\gamma_0 \sim 0.1$, and $\gamma_2 \sim -0.02$ eV, such corrections are generally small. The leading $O(v_4)$ corrections, in particular, may conveniently be included in $\mathcal{H}_n$ if one sets $\epsilon_0^u = u/2$, $\epsilon_1^u = (1 - z_2)/(u/2 + 2\kappa r_4 \omega_0)$ and $\epsilon_2^u = (1 - z_2)/u/2 + 4\kappa(1 + \kappa^2) r_4 \omega_0$, with $2\kappa r_4 \sim 0.005$ and $4\kappa(1 + \kappa^2) r_4 \sim 0.01$. Unlike $u$, such $O(v_4)$ corrections are common to the $K$ and $K'$ valleys and lead to weak electron-hole asymmetry. The relative magnitude of $(\epsilon_0^u, \epsilon_1^u, \epsilon_2^u)$ may vary with bias $u$ and can potentially control a valley rotation for small $u$. Still the orbital splitting among $\{\epsilon_\sigma^u\}$ is generally larger than the splitting among $\{\epsilon_n^u\}$, and the PZM sector will essentially maintain the spectra shown in Fig. 3. The electron-hole symmetric spectra there will also serve as the base point for further examining possible effects of nonleading intra- and interlayer parameters.

VI. SUMMARY AND DISCUSSION

In a magnetic field graphene trilayers acquire, on topological grounds, a special multiplet of nearly-zero-energy Landau levels with a threefold degeneracy in Landau orbitals. In this paper we have studied the structure of this PZM multiplet in $ABC$-stacked trilayer graphene and pointed out that its orbital degeneracy is lifted by quantum fluctuations of the valence band. Here we encounter a trilayer generalization of the “orbital” Lamb shift, discussed earlier for bilayer graphene. The splitting among the shifted energies $\{\epsilon_n^u\}$ acts as a quantum orbital breaking that generally exceeds intrinsic spin or valley breaking in scale, and essentially governs the structure of the PZM sector.

The orbital Lamb shift of the PZM Landau levels is a “field-theoretic” vacuum effect but is intimately correlated with the Coulomb interaction acting within the multiplet. This is because they have to combine to yield an electron-hole symmetric spectrum for the PZM multiplet (with only the leading couplings $\gamma_0$ and $\gamma_1$ kept) as a whole. In particular, large Coulombic gaps, expected at $\nu = 0$ and $\pm 3$, are essentially given by the energy scale $\sim 2\epsilon_\sigma^u$ of the orbital Lamb shift.

The PZM levels get mixed via the Coulomb interaction and avoid level crossing, keeping smaller orbital gaps (of magnitude $\sim 0.5 \tilde{V}_c$), as we have seen in Sec. V. Level crossing, if present, would enhance the degree of degeneracy and the steps of Hall plateaus would jump accordingly. Observations of possible $\nu = \pm 1, \pm 2, \pm 4, \pm 5$ quantum Hall states in high-quality samples, such as suspended or BN-supported ones, under high magnetic fields, if achieved, would be direct evidence for the presence of orbital mixing without level crossing. It is also possible, in principle, to detect the orbital gaps via cyclotron resonance within the PZM sector.

In this paper we have focused on $ABC$-stacked trilayer graphene. We remark that our analysis and conclusion cannot simply be carried over to the case of $ABA$ trilayers, which lacks a direct link between the $K$- and $K'$-valley expressions [such as Eq. (2)] and which thus requires a separate analysis.

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Appendix A: Derivation of Eq. (21)

In this appendix we present a proof of the completeness relation $\sum_{n=0}^{\infty} |g_{kn}^{n\sigma}|^2 = e^{\epsilon^2 p^2/2} \delta^{km}$ in Eq. (21). A simpler version of it is the following:

$$\sum_{n=0}^{\infty} f_{k-\mathbf{p}}^{pn} f_{-\mathbf{p}}^{np} = e^{\epsilon^2 p^2/2} \delta^{km} \tag{A1}$$

for integers $k, m \geq 0$, which is verified by use of the explicit form of $f_{k-\mathbf{p}}^{pn}$ in Eq. (14). We show that Eq. (21) is essentially reduced to Eq. (A1).

Let us first look at Eq. (13) and put the (orthonormal set of) six eigenvectors of $\mathcal{H}_n$ for each $n \in (3, 4, \ldots)$ into the orthogonal matrix $T_n = (v_{n1}, v_{n2}, \ldots, v_{n6})$ with $|n_n| = n$ and $\sigma \in (1, 2, \ldots, 6)$. The first row of $T_n$ is $(b_{n1}^{(1)}, b_{n2}^{(1)}, \ldots, b_{n6}^{(1)}) \equiv \{b_n^{(1)}\}$, the second row is $\{d_n^{(1)}\}$, etc. These row vectors also form an orthonormal basis. This feature is also true for $n \in (0, 1, 2)$, except that $T_n$ has a smaller rank.

In taking the product $\sum_{n} g_{k-\mathbf{p}}^{kn} g_{-\mathbf{p}}^{nm}$ one may first sum over $n$, for each fixed $n = |n_n|$. One thereby encounters inner products of the row vectors such as $\sum_{\sigma} \{b_{n}^{(1)}\}\{b_{n}^{(1)}\} = \delta^{ij}$ and $\sum_{\sigma} \{b_{n}^{(i)}\}\{d_{n}^{(j)}\} = 0$. The remaining sum over $|n|$ is essentially reduced to formula (A1) and one eventually finds that $\sum_{n} g_{k-\mathbf{p}}^{kn} g_{-\mathbf{p}}^{nm} = e^{\epsilon^2 p^2/2} \delta^{km} (v_{k} \cdot v_{m})$, which leads to Eq. (21).
