Trigonal warping and Berry’s phase $N\pi$ in ABC-stacked multilayer graphene

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The electronic band structure of ABC-stacked multilayer graphene is studied within an effective mass approximation. The electron and hole bands touching at zero energy support chiral quasiparticles characterized by Berry’s phase $N\pi$ for $N$-layers, generalizing the low-energy band structure of monolayer and bilayer graphene. We investigate the trigonal-warping deformation of the energy bands and show that the Lifshitz transition, in which the Fermi circle breaks up into separate parts at low energy, reflects Berry’s phase $N\pi$. It is particularly prominent in trilayers, $N=3$, with the Fermi circle breaking into three parts at a relatively large energy that is related to next-nearest-layer coupling. For $N=3$, we study the effects of electrostatic potentials which vary in the stacking direction, and find that a perpendicular electric field, as well as opening an energy gap, strongly enhances the trigonal-warping effect. In magnetic fields, the $N=3$ Lifshitz transition is manifested as a coalescence of Landau levels into triply-degenerate levels.

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I. INTRODUCTION

Soon after the fabrication of individual graphene flakes a few years ago\textsuperscript{1}, it was realized that low-energy quasiparticles in graphene are chiral, with a linear dispersion and degree of chirality characterized by Berry’s phase $\pi$ in monolayer graphene\textsuperscript{2,3} and quadratic dispersion related to Berry’s phase $2\pi$ in bilayers\textsuperscript{4,5}. In addition to their degree of chirality, bilayers are distinguished from monolayers by the possibility of using doping or external gates to induce interlayer asymmetry that opens a tunable gap between the conduction and valence bands\textsuperscript{6,7,8,9,10,11}, as observed in transport\textsuperscript{12,13} and spectroscopic measurements\textsuperscript{14,15,16,17,18,19}.

Recently, there has been experimental interest in the transport properties of trilayer graphene\textsuperscript{20,21,22}. It is expected that two different types of stacking order, ABA and ABC (illustrated in Fig. 1), will be realized in nature and that electronic properties will depend strongly on the stacking type. For ABA-stacked trilayer graphene, the low-energy electronic band structure consists of separate monolayer-like and bilayer-like bands\textsuperscript{23,24,25,26,27} that become hybridized in the presence of interlayer asymmetry\textsuperscript{28,29}. By contrast, the low-energy bands of ABC-stacked trilayers\textsuperscript{6,10,23,28} do not resemble those of monolayers or bilayers, but appear to be a cubic generalization of them. Thus, there is a cubic dispersion relation and chirality related to Berry’s phase $3\pi$\textsuperscript{30,31}, and, as in bilayers, the application of interlayer asymmetry is predicted to open an energy gap in the spectrum\textsuperscript{7,10}.

In this paper, we show that the low-energy band structure of ABC-stacked multilayer graphene is not just a straightforward generalization of that of monolayers and bilayers. We focus on a particular aspect of the band structure, trigonal warping, which plays a crucial role in the low-energy band structure. Trigonal warping is a deformation of the Fermi circle around a degeneracy point\textsuperscript{32}, at each of two inequivalent corners of the hexagonal Brillouin zone that are known as $K$ points\textsuperscript{32} [Fig. 1(b)]. In bilayer graphene, trigonal warping is enhanced by the interlayer coupling and leads to a Lifshitz transition\textsuperscript{33} when the Fermi line about each $K$ point is broken into several pockets\textsuperscript{5,24,26,34,35,36,37,38}. Here, we develop an effective Hamiltonian for ABC-stacked trilayer graphene, to show that trigonal warping in it is both qualitatively and quantitatively different from that in bilayers. The main contribution to trigonal warping arises from a different type of interlayer coupling that is missing in bilayers and we predict that it leads to a Lifshitz transition at a much larger energy $\sim 10\text{meV}$, which is 10 times as large as in a bilayer. Moreover, on undergoing the Lifshitz transition, the Fermi surface breaks into a different number of pockets reflecting Berry’s phase $3\pi$ in contrast to $2\pi$ in bilayers. Here, we also generalize our approach to describe trigonal warping in general ABC-stacked $N$-layer graphene, to show that Berry’s phase $N\pi$ manifests itself in different characteristics of the Lifshitz transition.

In the next Section, we describe the effective mass model of ABC-stacked trilayer graphene and the resulting band structure. Then, in Section III we derive an effective low-energy Hamiltonian and we use it to compare the behavior of low-energy chiral quasiparticles in trilayers with those in monolayer and bilayer graphene. In Section IV, we provide an approximate analytical description of the Lifshitz transition in the absence and in the presence of interlayer asymmetry that opens a gap in the spectrum. Section V describes the manifestation of the Lifshitz transition in the degeneracy of Landau levels in the presence of a finite magnetic field. In Section VI we generalize our approach to ABC-stacked $N$-layer graphene. Throughout, we compare the approximate description of the effective low-energy Hamiltonian with numerical diagonalization of the full effective mass model.
layer coupling between sites or below each other, parameter $\gamma_B = i$ Weis-McClure parameterization of tight-binding coupling within each layer is described by $\gamma_1$ coupling between sites $B3$ and $A1$ in different unit cells.

**II. THE EFFECTIVE MASS MODEL OF ABC-STACKED TRIAYER GRAPHENE**

The lattice of ABC-stacked trilayer graphene consists of three coupled layers, each with carbon atoms arranged on a honeycomb lattice, including pairs of inequivalent sites $\{A1, B1\}$, $\{A2, B2\}$, and $\{A3, B3\}$ in the bottom, center, and top layers, respectively. The layers are arranged as shown in Fig. 1(a,c), such that pairs of sites $B1$ and $A2$, and $B2$ and $A3$, lie directly above or below each other [for comparison, the unit cell of ABC-stacked graphene is shown in Fig. 1(d)]. In order to write down an effective mass Hamiltonian, we adapt the Slonczewski-Weiss-McClure parameterization of tight-binding couplings of bulk graphite [39]. Nearest-neighbor ($A_i$-$B_i$ for $i = \{1, 2, 3\}$) coupling within each layer is described by parameter $\gamma_0$, $\gamma_1$ describes strong nearest-layer coupling between sites ($B1$-$A2$ and $B2$-$A3$) that lie directly above or below each other, $\gamma_3$ describes weaker nearest-neighbor coupling between sites $A1$-$B2$ and $A2$-$B3$ ($A1$-$A2$, $B1$-$B2$, $A2$-$A3$, and $B2$-$B3$). With only these couplings, there would be a degeneracy point at each of two inequivalent corners, $K_{\pm}$, of the hexagonal Brillouin zone [32] but this degeneracy is broken by next-nearest-layer coupling $\gamma_2$, between sites $A1$ and $B3$ that lie on the same vertical line [11] [23] [28]. For typical values of bulk ABA graphite we quote $[39] \gamma_0 = 3.16eV$, $\gamma_1 = 0.39eV$, $\gamma_2 = -0.020eV$, $\gamma_3 = 0.315eV$ and $\gamma_4 = 0.044eV$. Although the atomic structures of ABA and ABC (rhombohedral) graphite are different, we refer to those values in the following numerical calculations, assuming that the corresponding coupling parameters have similar values [40].

In a basis with atomic components $\psi_{A1}$, $\psi_{B1}$, $\psi_{A2}$, $\psi_{B2}$, $\psi_{A3}$, $\psi_{B3}$, the ABC-stacked trilayer Hamiltonian [7, 28, 40, 41] is

$$\hat{H}_{ABC} = \begin{pmatrix} D_1 & V & W \\ V^\dagger & D_2 & V \\ W^\dagger & V^\dagger & D_3 \end{pmatrix},$$

where the $2 \times 2$ blocks are

$$D_i = \begin{pmatrix} U_i & v \pi \dagger \\ v \pi & U_i \end{pmatrix} \quad (i = 1, 2, 3),$$

$$V = \begin{pmatrix} -v_4 \pi \dagger & v_3 \pi \\ v_3 \pi & v_4 \pi \dagger \end{pmatrix}, \quad W = \begin{pmatrix} 0 & \gamma_2/2 \\ \gamma_1 & 0 \end{pmatrix},$$

where $v = (\sqrt{3}/2)\alpha\gamma_0/h$, $v_3 = (\sqrt{3}/2)\alpha\gamma_3/h$, $v_4 = (\sqrt{3}/2)\alpha\gamma_4/h$, $\pi = \xi p_x + ip_y$, $\pi^\dagger = \xi p_x - ip_y$, and $\xi = \pm 1$ is the valley index. Here $p = (p_x, p_y) = p(\cos \phi, \sin \phi)$ is the momentum measured with respect to the center of the valley [Fig. 1(b)]. The parameters $U_1$, $U_2$, and $U_3$ describe on-site energies of the atoms on the three layers that may be different owing to the presence of substrates, doping, or external gates. In the following, we set the average on-site energy to zero $U_1 + U_2 + U_3 = 0$ and write differences between the on-site energies in terms of asymmetry parameters $\Delta_1$ and $\Delta_2 [26].$

$$\Delta_1 = (U_1 - U_3)/2,$$

$$\Delta_2 = (U_1 - 2U_2 + U_3)/6.$$

Parameter $\Delta_1$ describes a possible asymmetry between the energies of the outer layers, whereas $\Delta_2$ takes into account the possibility that the energy of the central layer may differ from the average outer layer energy. As there are six atoms in the unit cell, ABC-stacked trilayer graphene has six electronic bands at low energy as plotted in Fig. 2. For no interlayer asymmetry $\Delta_1 = \Delta_2 = 0$, and exactly at the K point, $p = 0$, the eigenvalues $\epsilon$ of Hamiltonian Eq. 1 are given by $(\epsilon^2 - \gamma_1^2)^2(\epsilon^2 - \gamma_2^2/4) = 0$. Four of the bands are split away from zero energy by interlayer coupling $\gamma_1 (\epsilon = \pm \gamma_1$ twice). These high-energy bands correspond to dimer states formed primarily from orbitals on the atomic sites $B1$, $A2$, $B2$, and $A3$ that are strongly coupled by $\gamma_1$. The other two bands ($\epsilon = \pm \gamma_2/2$) are split slightly away from zero energy by next-nearest layer coupling $\gamma_2/2$ that connects atomic sites $A1$ and $B3$ [10, 23, 28].

Figure 2 shows the band structure at several $\Delta_1$‘s with $\Delta_2 = 0$, using the parameter values quoted above. $\Delta_1$ opens an energy gap between the lower electron and hole bands, because of the energy difference between A1 and
begin with the energy eigenvalue equation

dimer components

the six-component Hamiltonian, Eq. (1), eliminate the

simplify the expressions for low-energy components

θ

stacked trilayer graphene [7] for

has been applied to bilayer graphene [5] and to ABC-

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ABC-stacked trilayer graphene it is useful to derive an

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electron band at (a) ∆1/γ1 = 0 and (b) 0.4, showing that

the band is trigonally warped, and the contour splits into

three pockets at low energy. The detailed band structure

FIG. 2: Band dispersion of ABC-stacked trilayer graphene

in the vicinity of K± along p± axis. Parameter values are

γθ = 3.16eV, γ2 = 0.39eV, γ3 = −0.020eV, γ3 = 0.315eV and

γ4 = 0.044eV [39].

B3 sites [7, 11]. Figure 3 shows contour plots of the lower
electron band at (a) ∆1/γ1 = 0 and (b) 0.4, showing that

the band is trigonally warped, and the contour splits into

three pockets at low energy. The detailed band structure

III. THE LOW-ENERGY EFFECTIVE

HAMILTONIAN

To describe the low-energy electronic properties of
ABC-stacked trilayer graphene it is useful to derive an
effective two-component Hamiltonian that describes hopp-
ing between atomic sites A1 and B3. Such a procedure
has been applied to bilayer graphene [39] and to ABC-
stacked trilayer graphene [7] for γ3 = γ2 = ∆2 = 0. We begin
with the energy eigenvalue equation HΨ = εΨ of the six-
component Hamiltonian, Eq. 11, eliminate the dimer components χ = (ψB1, ψA2, ψB2, ψA3)T and, then,
simplify the expressions for low-energy components θ = (ψA1, ψB3)T by treating interlayer coupling γ1 as a large
energy scale [ε, vp, γ2, |γ3|, |γ4|, |∆1|, |∆2|] ≪ γ1. We denote hθ as the diagonal block of Hamiltonian of Eq. 11

corresponding to θ, hχ as the four by four diagonal block
corresponding to χ, and n as the off-diagonal 2 × 4 block
coupling θ and χ. The Schrödinger equation for θ can be
expanded up to first order in ε as [hθ − uhχ−1u]θ = εSθ

with S = 1 + uhχ−2u. Then, the effective Hamiltonian for

θ = S1/2θ becomes H(θ) = S−1/2[hθ − uhχ−1u]S−1/2.

Thus, we find the following two-component Hamilto-
nian in a basis of the A1-B3 sites:

\begin{align}
\hat{H}_A^{(\text{eff})} &= \hat{H}_3 + \hat{H}_{3c} + \hat{H}_{A1} + \hat{H}_{A2}, \\
\hat{H}_3 &= \frac{v^2}{\gamma_1} \begin{pmatrix} 0 & (\pi_1)^3 \\ \pi_1 & 0 \end{pmatrix}, \\
\hat{H}_{3c} &= \frac{2v v_3 p_2^2 + \gamma_2}{\gamma_1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\
\hat{H}_{A1} &= \Delta_1 \begin{pmatrix} 1 - v^2 p_1^2 & 0 \\ 0 & -1 \end{pmatrix}, \\
\hat{H}_{A2} &= \Delta_2 \begin{pmatrix} 1 - 3v^2 p_2^2 & 0 \\ 0 & 1 \end{pmatrix}.
\end{align}

Here we keep only the leading order for the terms including

γ2, v3 and v4. Terms H3 and \( \hat{H}_{A1} \) were derived in
Ref. [7]. The cubic term \( \hat{H}_3 \) describes effective hopping
between sites A1 and B3 via the other sites on the lattice.

FIG. 3: (a) Equi-energy contour plots of the lowest electron

band of ABC trilayer graphene at (a) ∆1 = 0 and (b) 0.4γ1.

Numbers on the contours indicate energy in units of γ1. Filled

and empty triangles represent local minima and maxima, re-

spectively, of the energy band.
that are strongly coupled by $\gamma_1$. Taken on its own, it produces a dispersion $\epsilon = \pm v^3 p^3 / \gamma^2_1$. $H_{3w}$ arises from the skewed interlayer coupling $\gamma_3$ and the next-nearest interlayer coupling $\gamma_2$, and is responsible for trigonal warping as discussed in detail later. $H_{3w}$, coming from another interlayer coupling $\gamma_4$, gives an identical curvature to the electron and hole bands and thus introduces electron-hole asymmetry. Terms $H_{\Delta_1}, H_{\Delta_2}$ arise from the interlayer asymmetries $\Delta_1$ and $\Delta_2$, respectively. $H_{\Delta_1}$ leads to the opening of an energy gap between the conduction and valence bands, while $H_{\Delta_2}$ produces a dispersion in a similar way as $H_{3w}$. In the two-component basis of $H_{AB}^\text{(eff)}$, time reversal is described by $\hat{H}^* (p, \Delta_1, \xi) = \hat{H} (-p, \Delta_1, -\xi)$ and spatial inversion by $\sigma_x \hat{H} (p, \Delta_1, \xi) \sigma_x = \hat{H} (-p, -\Delta_1, -\xi)$. Manes et al.\(^2\) showed that the Fermi points of ABC-stacked multilayers are stable with respect to the opening of a gap against perturbations that respect combined time reversal and spatial inversion, as well as translation invariance.

The low-energy effective Hamiltonian for ABC-stacked trilayer graphene bears some resemblance to that of bilayer graphene.\(^3\) In the lattice of bilayer graphene, Fig. 1(e), two of the sites (B1 and A2) are directly above or below each other and are strongly coupled by interlayer coupling $\gamma_1$ whereas two sites (A1 and B2) do not have a counterpart in the other layer. The low-energy Hamiltonian is written in a basis $(\psi_{A1}, \psi_{B2})$ of these two sites:

$$
\begin{align*}
\hat{H}_{\text{AB}}^\text{(eff)} &= \hat{H}_2 + \hat{H}_{3w} + \hat{H}_\Delta, \\
\hat{H}_2 &= -\frac{v^3}{\gamma_1} \begin{pmatrix} 0 & (\pi^1)^2 \\ \pi^2 & 0 \end{pmatrix}, \\
\hat{H}_{3w} &= v_3 \begin{pmatrix} 0 & \pi^1 \\ \pi^1 & 0 \end{pmatrix}, \\
\hat{H}_{2c} &= -\frac{2v^2 \gamma_3^2}{\gamma_1^2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\
\hat{H}_\Delta &= \Delta \left(1 - \frac{2v^2 \gamma_3^2}{\gamma_1^2}\right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\end{align*}
$$

where parameter $\Delta$ describes interlayer asymmetry between on-site energy $\Delta$ of the atoms, A1 and B1, on the first layer and $-\Delta$ of the atoms, A2 and B2, on the second layer.

The first term in each Hamiltonian, $\hat{H}_2$ for bilayers, Eq. 5, and $\hat{H}_3$ for ABC-stacked trilayers, Eq. 4, are members of a family of Hamiltonians $\hat{H}_J = F(p) \sigma \cdot n$ where $n = l_3 \cos(J \xi + \phi) + l_3 \sin(J \xi + \phi)$ for $p = p \cos(\phi) \sin(\phi) \xi$. They describe chiral quasiparticles, and the degree of chirality is $J = 1$ in monolayer graphene, $J = 2$ in a bilayer, and, here, $J = 3$ in ABC-stacked trilayer. Quasiparticles described by the Hamiltonians $\hat{H}_J$ acquire a Berry’s phase $-i \oint_C dp \cdot (\Psi^\dagger \nabla_p \Psi) = J \xi$, upon an adiabatic propagation along an equi-energetic line $C$. Thus charge carriers in ABC-stacked trilayer graphene are Berry’s phase $3\xi\pi$ quasiparticles, in contrast to Berry’s phase $\xi\pi$ particles in monolayers, $2\xi\pi$ in bilayers. As well as the first term in the Hamiltonian Eq. 4 of ABC-trilayers being a generalization of that in bilayers, the influence of interlayer asymmetry $\Delta = (U_1 - U_3)/2$ as described by $H_{\Delta}$ is similar to that in bilayers as described by $H_\Delta$, Eq. 5.

### IV. TRIGONAL WARPING AND THE LIFSHITZ TRANSITION

In a similar way to bulk graphite, the parameter $\gamma_3$ [where $v_3 = \sqrt{3}/2 \gamma_1 / h$] produces trigonal warping in bilayer graphene,\(^4\), where the equi-energetic line around each valley is stretched in three directions. This is due to the interference of the matrix elements connecting $A1$ and $B2$, where an electron hopping from $A1$ to $B2$ acquires a factor $e^{i2\xi\phi}$ in $\hat{H}_2$ and $e^{-i2\xi\phi}$ in $\hat{H}_{3w}$. We neglect the terms including $v_4$ which add a term $\propto p^2$ to the energy but don’t contribute to trigonal warping. At $\Delta = 0$, the eigenenergy of Eq. 5 is given by

$$
\epsilon \approx \pm \sqrt{v^3 p^2 - 2v_3 \gamma_3^2 p^3 / \gamma_1^3} \cos \phi + \frac{v^4 p^4}{\gamma_1^2}.
$$

The warping has a dramatic effect when $\hat{H}_2$ and $\hat{H}_{3w}$ have comparable amplitudes, i.e., $v^2 p^2 / \gamma_1 \approx v_3 p$, which is satisfied at $p \sim p_0 = \gamma_1 / v_3^2$. It leads to a Lifshitz transition\(^6\)\(^7\)\(^8\)\(^9\)^{2, 21, 29, 33, 43, 36, 46}, in which the equi-energetic line is broken into four separate pockets. There is one central pocket located around $p = 0$ and, three “leg” pockets centered at momentum of magnitude $p = p_0$ and angle $\phi_0 = 2\pi/3 + (1 - \xi)\pi/6$. The Fermi pocket separation occurs at energy $\epsilon_L = (v_3/v)^2 \gamma_1 / 4$, which is estimated to be $\epsilon_L \approx 1\text{meV}$.

In ABC-stacked trilayer graphene, there is a similar, but much greater warping effect. In hopping from $A1$ to $B3$, an electron acquires a factor $e^{i3\xi\phi}$ from $H_3$ and a factor of unity from $H_{3w}$, giving trigonal symmetry in $\phi$. At $\Delta_1 = \Delta_2 = 0$, the eigenenergy of Eq. 4 reads,

$$
\epsilon \approx \pm \sqrt{v^3 p^2 + 2v_3 \gamma_3^2 p^3 \cos \phi + g(p)^2},
$$

where $g(p) = \sqrt{v_3^2 p^2 / \gamma_1^2}$ comes from $H_3$ and $g(p) = -2v_3 \gamma_3^2 / \gamma_1 + \gamma_2 / 2$ from $H_{3w}$. Similarly to the bilayer, the warping effect is prominent when $|g(p)| \sim f(p)$, or $p \sim p_0$ with $v_0 \gamma_3 / \gamma_1 \approx (\gamma_1 / (2 \gamma_3))^{1/3} - (v_3 / v)^3$. This estimate is valid as long as $|v_3 / v| \lesssim |\gamma_1 / \gamma_3|^{1/3}$, which holds for typical parameter values of bulk graphite.

The major difference from the bilayer is the contribution of the parameter $\gamma_2 / 2$, which appears in the Hamiltonian without an accompanying momentum-dependent factor and, thus, it doesn’t vanish at $p = 0$. Such trigonal warping produces a Lifshitz transition at low energy, but, unlike bilayers, it occurs at energy $\epsilon_L \approx |\gamma_2 / 2|$. Although the value of $\gamma_2$ in ABC-trilayer graphene has not been measured experimentally, comparison with similar couplings in bulk graphite\(^3\) suggest that $|\gamma_2| \approx 20\text{meV}$.
This opens up the possibility that the Lifshitz transition in ABC-trilayer graphene could occur at a much higher energy than that in bilayers. At energy lower than $|\gamma_1|/2$, the contour splits into three leg pockets centered at $p \sim p_0$ in a trigonal manner. Unlike bilayer graphene, the central pocket is missing because $H_{xy}$ does not vanish at $p = 0$.

An effective Hamiltonian in the vicinity of the leg pockets, for $|p| \ll \varepsilon_L$, may be obtained by transforming to momentum $q = (q_x, q_y)$ measured from their centers,

$$q_x = p_x \cos \phi_0 + p_y \sin \phi_0 - p_0,$$

and $q_y = -p_x \sin \phi_0 + p_y \cos \phi_0$, (8)

and taking the limit of infinitely large $\gamma_1$:

$$\hat{H}_{ABC}^{\text{leg}} = 3\varepsilon \left| \frac{\gamma_1}{2\gamma_1} \right|^{2/3} \begin{pmatrix} 0 & \xi \alpha q_x - i q_y \\ \xi \alpha q_x + i q_y & 0 \end{pmatrix}. \tag{10}$$

where $\alpha = 1 + (4v_0/3v)(2\gamma_1/\gamma_2)^{1/3}$. Thus, the pockets are elliptical with dispersion $\epsilon \approx \pm 3|\gamma_1/(2\gamma_2)|^{2/3} v \sqrt{\alpha^2 q_x^2 + q_y^2}$. The different nature of the Lifshitz transition in bilayers and ABC-stacked trilayers is a manifestation of Berry’s phase in trilayer graphene, the geometrical phase integrated around the equi-energy line of each pocket is $\xi \pi$ as in a monolayer, giving $3\xi \pi$ in total. This is different from bilayers, where $3\xi \pi$ arises from three leg pockets and $-\xi \pi$ from the center pocket gives $2\xi \pi$ in total $[23, 57]$.

Interlayer asymmetry $\Delta_1$ opens a gap in the spectrum and produces a Mexican hat feature in the low-energy dispersion. [23] The eigenenergy corresponding to Eq. (11) is given by

$$\epsilon \approx \pm \sqrt{f(p)^2 + 2\xi f(p) g(p) \cos \phi + g(p)^2 + h(p)^2}, \tag{11}$$

with an extra term as compared to Eq. (11), $h(p) = \Delta_1(1-v^2p^2/\gamma_1^2)$, coming from $\hat{H}_{\Delta_1}$. For no trigonal warping $g(p) = 0$, it yields $\epsilon^2 = \Delta_1^2(1-v^2p^2/\gamma_1^2)^2$. The energy is $\epsilon = \pm \Delta_1$ at zero momentum, but there is a minima located isotropically about the center of the valley at finite momentum $p = p_1 \approx (2/3)^{1/4} \sqrt{\Delta_1 \gamma_1^3}/v$ (for $|\Delta_1| \ll |\gamma_1|$) at which the energy is $\epsilon = \epsilon_1 \approx \pm \Delta_1 (1 - (2/3)^{3/2}|\Delta_1/\gamma_1|)$.

In the presence of trigonal warping, there is an interplay between the Mexican hat feature and the Lifshitz transition. In the large gap regime, such that $|g| \ll f, h$, the circular edge of the band bottom is trigonally distorted by the perturbation of $g(p)$, making three pockets on it. The bottom of the pockets moves to momentum $p = p_1 + \delta p_1$ with $\delta \phi_1/\gamma_1 \approx (v^2/8)(2\Delta_1/\gamma_1^2) - (5/6)(\varepsilon_L/v)$, and energy $\epsilon = \epsilon_1 - \delta \epsilon_1$ with $\epsilon_1 = (2/3)^{3/4} \sqrt{\Delta_1 \gamma_1^3}/2 - \sqrt{8/3}(\varepsilon_L/v)\Delta_1$. The area of the pocket in k-space becomes of the order of $p_1 \delta p_1$, and the depth in energy is of order $\delta \epsilon_1$, both of which increase as $\Delta_1$ increases. This significant enlargement of the trigonal pockets, in the presence of finite $\Delta_1$, is illustrated in Figure 3 which is produced by numerical diagonalization of the full Hamiltonian Eq. (11). Note that similar widening of the pockets by the gap term occurs in bilayer graphene as well. This can be understood in an analogous way, by writing $f(p) = v^2p^2/\gamma_1$, $g(p) = v_3p$, and $h(p) = \Delta(1-2v^2p^2/\gamma_1^2)$.

V. LANDAU LEVEL SPECTRUM

The energy levels in a magnetic field are given by replacing $p$ with $p + eA$ in the Hamiltonian Eq. (11), where $A(r)$ is the vector potential corresponding to the magnetic field. Here we consider a uniform magnetic field $B$ applied along $+z$ direction in a Landau gauge $A = (0, Bx)$. Operators $\pi$ and $\pi^\dagger$ are then related to raising and lowering operators $a^\dagger$ and $a$ of the Landau level in a conventional two-dimensional system, such that $[\pi^\dagger/\sqrt{2}\hbar]|\pi| = a^\dagger$ and $a$ for $K_+$ and $K_-$ respectively, with $\pi = \sqrt{B/\hbar}.E$. The operator $a$ acts as $a|\varphi_n,k\rangle = \sqrt{\Delta}\varphi_{n-1,k}$, and $a|\varphi_0\rangle = 0$, where $\varphi_{n,k}(x, y) \propto e^{ik\rho e^{-z^2/2H_B}}$ is the wavefunction of the $n$th Landau level in a conventional two-dimensional system with $z = (x + kiB)/\hbar$, and $H_B$ being a Hermite polynomial.

In the simplest model including only $\gamma_1$ and $\gamma_2$ without trigonal warping, the effective Hamiltonian $H_3$ in Eq. (11) yields the eigenstates for $K_+$ [7]

$$\epsilon_n = 0, \quad \Psi_{nk} \propto \begin{cases} \varphi_{n,k} \\ 0 \end{cases} \quad (n = 0, 1, 2),$$

$$\epsilon_n = \frac{s^3}{\gamma_1^3} \sqrt{n(n-1)(n-2)} \quad (n \geq 3), \tag{12}$$

where $s = \pm 1$ describes the electron and hole levels, respectively. $\Delta_1 = \sqrt{2}h^2e^2B$. The eigenstates $n = 0, 1, 2$ have a non-zero amplitude only on the first element $(A1)$, and remain at zero energy regardless of the magnetic field strength, while the energy of the other levels behaves as $\propto B^{3/2}$. At the other valley $K_-$, there is a similar structure except that the first and second elements are interchanged, i.e., the zero-energy Landau levels have amplitudes only on sites $B3$ [7].

Trigonal warping gives a remarkable feature in the structure of Landau levels. In enough small fields, the three leg pockets independently accommodate a nearly equal number of Landau levels so that they are triply degenerate. This is in contrast to bilayer graphene where the central pocket also contributes to the degeneracy [4]. The low-energy effective Hamiltonian, Eq. (11), shows that the Landau level energy follows a similar sequence as that in monolayer graphene, $\epsilon_n = 3|\gamma_2/(2\gamma_1)|^{2/3} \sqrt{\alpha \Delta_B \text{sgn}(n)}\sqrt{n}$ where $n$ is integer. The total number of Landau levels accommodated in each pocket is roughly estimated by the condition $\epsilon_n \sim |\gamma_2|/2$, as $n \sim (\gamma_1/\Delta_B)^2|\gamma_2/(2\gamma_1)|^{2/3}/(9\alpha)$. 


Fig. 4(a) shows the Landau level spectrum at the valley $K_+$ as a function of $\Delta_B(\propto \sqrt{B})$, numerically calculated for the full parameter model Eq. (11) at $\Delta_1 = \Delta_2 = 0$. Below $\epsilon = \gamma_2/2$, the Landau levels are triply degenerate and move in proportion to $\sqrt{B}$. The degeneracy of each level is broken at $\epsilon = \gamma_2/2$, and it splits into three separate levels, corresponding to coalescence of the leg pockets at the Lifshitz transition. At even higher energy, it approaches $B^{3/2}$ behavior as described in Eq. (12). The triply degenerate level around zero energy is regarded as the $n = 0$ level in each of three pockets. In actual fact, its degeneracy is split slightly in a large magnetic field, owing to magnetic break down among the semiclassical orbits in the leg pockets, which is caused by the parameter $v_4$. When the trigonal warping vanishes, those three levels switch to the degenerate levels with indices $n = 1, 2, 3$.

Fig. 4(b) shows the Landau level spectrum at $K_+$ as a function of asymmetry $\Delta_1$ with fixed magnetic field $\Delta_B = 0.1\gamma_1 (B \sim 1T)$. As $\Delta_1$ is changed from negative to positive, three Landau levels [indicated by the single diagonal line that crosses $\epsilon = 0$ at $\Delta_1 = 0$ in Fig. 4(b)] are pumped from the hole side to the electron side. In the approximate model of Eq. (12), this corresponds to the fact that the energy levels $n = 0, 1, 2$ have a wave amplitude only on $A1$, so that it acquires on-site energy $+\Delta_1$ in the first order of perturbation. At the other valley $K_-$, there is the opposite movement, i.e., the three levels go down from positive to negative energies in increasing $\Delta_1$.

The energy of the Lifshitz transition appears as a region where the levels are densely populated, and below that energy the levels are triply degenerate [indicated by the shaded region in Fig. 4(b)]. It should be noted that the number of triply-degenerate levels increases for larger $\Delta_1$, reflecting the enlargement of the trigonal pockets discussed above. In a measurement of Hall conductivity, those triply-degenerate Landau levels would be observed as quantum Hall steps of magnitude $3g_v g_s e^2/h$, where $g_v = g_s = 2$ are the valley and spin degeneracies, respectively.

**VI. GENERAL ABC-STACKED MULTILAYER GRAPHENE**

The analysis of ABC-stacked trilayer graphene can be extended to multilayers with $N$ layers. We consider each layer to consist of carbon atoms on a honeycomb lattice, and the layers are arranged with ABC stacking. The Hamiltonian is written in a basis $\psi_{A1}$, $\psi_{B1}$, $\psi_{A2}$, $\psi_{B2}$, $\cdots$, $\psi_{AN}$, $\psi_{BN}$, as

$$\hat{H}_N = \begin{pmatrix} D_1 & V & W \\ V^\dagger & D_2 & V \\ W^\dagger & V^\dagger & D_3 & \cdots \\ & \ddots & \ddots \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots & \ddots \end{pmatrix},$$

where the $2 \times 2$ blocks $D_i$, $V$, $W$ are defined in Eqs. (13). Pairs of sites $B(i)$ and $A(i + 1)$ ($i = 1, \cdots, N - 1$) are vertically above or below each other, and are strongly coupled by $\gamma_1$ giving dimer states. Thus, all the sites in the lattice, except two, contribute to bands that lie away from zero energy. The remaining two sites, $A_1$ and $B_N$, form the lowest-energy electron and hole bands.
Note that these sites lie on the outer layers, so that the lowest bands are missing in an infinite system with periodic boundary conditions applied in the stacking direction. The band structure has triongol symmetry for any \( N \). This is checked by applying the transformation \( \phi \to \phi + 2\pi/3 \) to Eq. (13), where the change in the matrix elements can be canceled by the gauge transformation \( \psi_n = e^{-i \gamma_1 \pi} \psi_n \), with \( \gamma_n = e^{-i 2\pi n/3} \).

The effective low-energy Hamiltonian is obtained by treating terms other than \( \gamma_1 \) as perturbations. The effective Hamiltonian in a basis \( \{ \psi_A, \psi_B \} \) reads

\[
\hat{H}_N^{(\text{eff})} = \begin{pmatrix} 0 & X(p) \\ X(p) & 0 \end{pmatrix} + \frac{2vu_4p^2}{\gamma_1^2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},
\]

\[
X(p) = \sum_{\{n_1, n_2, n_3\}} \frac{(n_1 + n_2 + n_3)!}{n_1!n_2!n_3!} \frac{1}{(-\gamma_1)^{n_1+n_2+n_3}} \epsilon_{\alpha\beta\gamma}(vpe^{-i\xi\phi}n_1)(v_3pe^{-i\xi\phi}n_2) \left( \frac{\gamma_2}{2} \right)^{n_3},
\]

where the summation is taken over positive integers which satisfy \( n_1 + 2n_2 + 3n_3 = N \). Here we collected all the higher order terms not including \( v_4 \), but retain just the leading term for \( v_4 \). The trigonal warping structure can be described well in this treatment as shown below, since \( v_4 \) only gives the circularly-symmetric band curvature as in ABC trilayer.

The eigenenergies are given by \( \epsilon = 2vu_4p^2/\gamma_1^2 \pm |X(p)| \). If we neglect \( \gamma_2 \) and \( v_3 \), we have \( X = (\epsilon vpe^{i\xi\phi})^N / (-\gamma_1)^{N-1} \) which gives a pair of bands, isotropic in momentum, which touch at the origin \( \mathbf{29, 30} \). Berry’s phase integrated along an energy contour is \( N\xi\pi \) at every energy. Perturbation by \( \gamma_2 \) and \( v_3 \) produces trigonal warping as observed in the trilayer. Figure 5 shows the lower energy band structure for \( \phi = 0 \) at several \( N \)'s, where the solid lines are calculated using the original Hamiltonian Eq. (13), and the dashed lines use Eq. (14). We can see that the effective Hamiltonian reproduces the original band structure rather well including the positions of the band touching points, except that the magnitude in energy tends to be overestimated around \( vp \sim \xi \) where the perturbative approach fails.

The band touching points, or Dirac points, are given by the solution of \( X(p) = 0 \). They appear in a series of \( p \)'s at only three angles \( \phi_0 = 2n\pi/3 + (1 - \xi)\pi/6 \), and around which the Hamiltonian has a chiral structure similar to monolayer graphene. We empirically found that the arrangement of these points obeys the following rules: We have \( \lfloor (N + 1)/3 \rfloor \) Dirac points at \( p \neq 0 \) at each of three angles, and each of them has Berry’s phase \( \xi \pi \). Here \( \lfloor x \rfloor \) represents the greatest integer which does not exceed \( x \). The Dirac point at the center \( (p = 0) \) only appears when \( N \) is not a multiple of 3, and its Berry’s phase is \( \xi \pi \) and \( -\xi \pi \) when \( N = 1 \) and \( -1 \) (mod 3) respectively. The total Berry’s phase summed over all Dirac points is always \( N\xi\pi \), the same as the value without trigonal warping. The energy scale for fine structure around the Dirac points becomes smaller as \( N \) increases, because the matrix elements connecting \( A_1 \) and \( B_N \) become higher order in \( p \) for larger \( N \). We see that \( N = 3 \) has the most prominent structure, where \( \gamma_2 \) directly connects \( A_1 \) and \( B_N \). The parameter \( v_4 \) never opens a gap at the Dirac points but gives an energy shift by \( 2vu_4p^2/\gamma_1^2 \) associated band curvature, leading to misalignment of the Dirac point energies as shown in Fig. 5. The curvature is independent of \( N \) because it is due to the second order process from \( A_1 \) or \( B_N \) to the nearest-neighboring dimer state.

The approach applied to the Landau levels of the trilayer in Sec. [V] can be extended to the \( N \)-layer case. In the simplest model including only \( \gamma_0 \) and \( \gamma_1 \), the Landau...
levels at $K_+$ read

$$
\epsilon_n = 0, \quad \psi_{nk} \propto \left( \varphi_{n,k} \right) (n = 0, 1, \cdots, N - 1), \quad (15)
$$

$$
\epsilon_{sn} = s \frac{\Delta_B^N}{\gamma (N-1)} n(n-1) \cdots (n-N+1) \quad (n \geq N), \quad (16)
$$

with $s = \pm 1$. The first and second elements are again interchanged at the other valley $K_-$. The zero-energy level is now $N$-fold degenerate per valley and per spin [7, 29, 30]. In presence of trigonal warping and $v_4$, however, this is expected to split in accordance with the discrepancy between the energies of different Dirac points shown in Fig. 5 for $B = 0$, while some levels keep three-fold degeneracy owing to trigonal symmetry as in the trilayer case. It is possible that electronic interactions may create exotic collective modes in such highly-degenerate Landau levels, but we leave the discussion of this for future studies.

VII. CONCLUSIONS

In ABC-stacked multilayer graphene with $N$ layers, two low-energy bands in the vicinity of each valley are formed from two electronic orbitals that lie on the bottom and top layers of the system. Such bands support chiral quasiparticles corresponding to Berry’s phase $N \pi$. The interplay between different types of interlayer coupling produces trigonal warping, in which the Fermi circle around each valley is stretched in three directions. At very low energy, trigonal warping leads to a Lifshitz transition [32] when the Fermi circle breaks up into separate pockets, in such a way that the total Berry’s phase is conserved. We predict that the Lifshitz transition is particularly prominent in trilayers, $N = 3$, with the Fermi circle breaking into three parts at a relatively large energy that is related to next-nearest-layer coupling.

VIII. ACKNOWLEDGMENTS

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