Magnetic Breakdown in Twisted Bilayer Graphene

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Introduction – The fundamental description of electron dynamics in a crystal and a uniform magnetic field involves orbital motion in a plane perpendicular to the field, along contours of constant energy [11, 2] as a function of crystal momentum $k$. This behavior can be significantly modified when tunneling from one trajectory to another becomes important, a phenomenon known as magnetic breakdown (MB) [3]. MB is important when the closest approach between $k$-space trajectories is on the order of the inverse of magnetic length, $l_B \approx 100/\sqrt{B}[\text{nm}]$, where $B$ is the magnetic field in Tesla. MB sometimes leads to the formation of open orbits, with dramatic transport signatures [1].

MB effects in bulk metals can be challenging to observe because saddle points in a band structure, where MB initially sets in as the electron energy changes [3], are often quite far from the Fermi energy. Recently, excellent candidates to observe MB phenomena have become available in the form of twisted graphene bilayers [6, 7] and graphene deposited on boron nitride substrates [8, 10]. These two-dimensional systems can support large unit cells in real space (“Moiré patterns”), and correspondingly small Brillouin zones, for which critical points in the energy dispersion can be at relatively low energy [11, 12]. Such large unit cells have allowed the recent observation of the self-similar Hofstadter spectrum [13–15] and graphene deposited on boron nitride substrates [8, 10]. These trajectories within a doubled Brillouin zone constitute a network in which an $S$-matrix at each saddle point is used to model tunneling between different layers. Matching of the semiclassical wavefunctions throughout the network determines the energy spectrum. Semiclassical orbits with energies well below that of the saddle points are Landau levels of the Dirac points in each layer. These continuously evolve into both electron-like and hole-like levels above the saddle point energy. Possible experimental signatures are discussed.

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Hamiltonian and Saddle Point Dispersions – Our starting point is the zero-field Hamiltonian

$$H = \left( \begin{array}{c} H_T \\ w \sum_{i=0,1,2} V_i \end{array} \right),$$

in which $H_{T,B} = v_F \left[ \hat{\sigma}_z p_1 + \hat{\sigma}_y (p_2 + \frac{k_B}{2}) \right]$ are the Dirac Hamiltonians for uncoupled top/bottom layers, with Dirac points located at $\mathbf{k} = (0, \pm \frac{\pi}{2})$, $p_{1,2}$ are components of the momentum operator, and the Pauli matrices $\hat{\sigma}_x,y,z$ act on the sublattice index. The coupling terms, $V_0 = i\hat{\alpha}_0$, $V_1 = i\hat{\alpha}_1 e^{iG_1 \cdot \mathbf{r}}$, and $V_i = i\hat{\alpha}_2 e^{iG_2 \cdot \mathbf{r}}$, are the largest interlayer hopping terms expected in a continuum model [12, 33]. These introduce discrete translational symmetry characterized by reciprocal lattice vectors $\mathbf{G}_{1,2} = k_0 (\pm \frac{\sqrt{3}}{2}, \frac{3}{2}) \equiv (\pm G_x, G_y)$. The hopping matrices are then specified by $\hat{\alpha}_0 = \hat{\delta}_1 + \hat{\sigma}_z, \hat{\alpha}_1 = \bar{\xi} e^{i\pi/2} \hat{\sigma}_z e^{-i\pi/2}$, and $\hat{\alpha}_2$ is the two-dimensional unit matrix, $z = e^{i\pi/2}$, and $\bar{\xi}$ is its complex conjugate.

To understand the behavior of this system, we treat the interlayer hopping as a weak periodic perturbation. This has important qualitative effects for nearly degenerate states in the top and bottom layers that are coupled by the perturbation. For example (see Fig. 1), a degeneracy between the top and bottom Dirac bands in the neighborhood of $M_a$ is split by the interlayer term $V_0$. Setting $v_F$ to unity, we find that the two states at $k = 0$ with energy $E = \frac{\hbar v_F}{2}$ in the absence of $V_0$ splits into states of energies $\sqrt{k_0^2 + 4v_F^2}/2 \pm w$. Near $M_a$, one may treat terms involving (small) momenta $\mathbf{k} = (k_x, k_y)$ perturbatively, to obtain a two-band effective Hamiltonian [34]

$$H_{sp} = (k_0/2 + k_1^2/k_0) \hat{\delta}_2 + \alpha (2k_1 + k_0) \hat{\sigma}_z - k_2 \hat{\sigma}_x,$$

where $\alpha = w/k_0$ is small. The eigenstates of $H_{sp}$ include a parabolic band at higher energy, and a lower band with a saddle point (SP) for which the dispersion is $E_{sp}(k_1, k_2) = k_0/2 + k_1^2/k_0 - \sqrt{(w + 2\alpha k_1)^2 + k_2^2}$, leading to a van Hove singularity at $E_{sp}(w, 0) = k_0/2 - w(1 + \alpha)$. This is similar to numerical results found in Ref. [33].

There are two other saddle points in the first BZ, near $M_b$ and $M_c$ in Fig. 1. Dispersions for these can be obtained in a way very similar to that of $M_a$ by employing an appropriate unitary transformation, shifting the zero of momentum for one of the two layers by $\mathbf{G}_1$ or $\mathbf{G}_2$. Up to 120° rotations, the resulting spectra are essentially identical to that of $M_a$.

Magnetic Translation (MT) Operators – To incorporate a uniform perpendicular magnetic field we introduce a vector potential $A = B(-y/2, x/2)$. To study the small $B$ limit it is convenient to work with momentum-space wavefunctions, so that the momentum operators $p_i$ entering Eq. 1 are replaced by $\Pi_{1,2} = k_{1,2} \pm \frac{1}{2\hbar} \partial_{k_{1,2}}$. In the momentum representation, the interlayer tunneling terms are $\hat{V}_i = i\tau_{1,2} (\mathbf{G}_i)$ where $\mathbf{G}_0 = 0$, with momentum translation operators $\tau_{\mathbf{G}}(\mathbf{G}) = e^{i\mathbf{G} \cdot \mathbf{k}}$. To exploit the translational symmetries of the problem we define MT operators

$$T_1(G_x) = \exp \left[ G_x \left( \partial_{k_1} - 2i\tau_B^2 k_2 \right) \right],$$

$$T_2(G_y) = \exp \left[ G_y \left( \partial_{k_2} + 2i\tau_B^2 k_1 \right) \right],$$

which commute with $\Pi_{1,2}$. The combinations $T(G_{1,2}) = T_1(\pm G_x)T_2(G_y)$ moreover commute with the full Hamiltonian, as well as with one another, if

$$4\tau_B^2 G_x G_y = 2\pi N,$$

for any integer $N$. We focus on magnetic fields satisfying this equality. Note such fields have the form $B_N = B/N$, so that our analysis applies to a dense set of small magnetic fields.

Eigenfunctions of the Hamiltonian can also be expressed as eigenfunctions of MT operators that commute with $H$, and it is convenient to choose the particular combination $T(G_1)T(G_2) = T_2^2(G_y)$ and $T(G_1)$ for this purpose. To see how this plays out, we consider spinor wavefunctions written in the form $\psi(k_1, k_2) = \int d\tilde{k} e^{-2i\tau_B^2 k_1 k_2 + 4i\tau_B^2 k_1 k_2} \tilde{\psi}(k_1, \tilde{k})$. In the absence of interlayer coupling, $\tilde{k}$ is a good quantum number and eigenfunctions of the Hamiltonian involve harmonic oscillator states whose centers lie near $k$. Thus $\tilde{k}$ can be viewed as a momentum-space guiding center coordinate. More generally, the requirement that wavefunctions be eigenvectors of $T_2^2(G_y)$ dictates that $e^{i\mathbf{G}_0 \cdot \mathbf{k}} \tilde{\psi}(k_1, \tilde{k})$ be the same for all the $\tilde{\psi}(k_1, \tilde{k})$’s entering a wavefunction. The integral

![FIG. 1: (Color online) Semiclassical orbits in the doubled BZ. Solid (red) trajectories are in top layer, dashed (blue) are on bottom. Circular orbits correspond to energies below star point, star-like (purple) orbits are above. Saddle points are labeled by $M_a, M_b, M_c$. Symbols of cross represent the Dirac points.](image-url)
over \( \tilde{k} \) then becomes a discrete sum. To see the effect of interlayer coupling one needs to notice that the action of momentum shift operator \( \tau(\hat{G}_1) \) appearing in the interlayer coupling on \( \tilde{\psi} \) becomes

\[
\tau(\hat{G}_1)\tilde{\psi}(k_1, \tilde{k}) = e^{-2i\tilde{\psi}(k_1-2\tilde{k})G_x}\tilde{\psi}(k_1 + G_x, \tilde{k} + G_x/2).
\]

This is consistent with the allowed discrete values of \( \tilde{k} \) for a given wavefunction provided Eq. 5 is obeyed.

Thus \( \tilde{\psi} \) can be written as a sum over wavefunctions \( \tilde{\psi}(k_1, \tilde{k}) \) with \( \tilde{k} = \tilde{k}_0 + \cdots \) and \( 0 \leq \tilde{k}_0 < G_x/2 \). The set of \( \tilde{k} \)'s one must retain is further reduced by use of a second MT symmetry condition, \( T(\hat{G}_3)\psi = e^{i\theta}\psi \). This becomes the condition \( e^{2i\tilde{\psi}_G(k_1 + G_x, \tilde{k} + G_x) = e^{i\theta}\tilde{\psi}(k_1, \tilde{k})} \). Ultimately one needs to only compute two functions, e.g., \( \tilde{\psi}(k_1, \tilde{k}_0) \) and \( \tilde{\psi}(k_1, \tilde{k}_0 + G_x/2) \).

Some comments are in order. First, the reduction of the wavefunction to two functions of \( k_1 \) was possible because of our gauge choice \[35\]. Secondly, since \( \tilde{\psi}(k_1, \tilde{k}) \) involves a single continuous variable, \( k_1 \), it can be approximated conveniently in a semiclassical approach. Because we need to retain two values of \( \tilde{k} \), these wavefunctions must be represented in two BZ’s \[35\]. Finally, while the two-BZ semiclassical description is strictly valid only for fields satisfying Eq. 6, we will treat \( B \) as a continuous variable. This captures the broad shape of the spectrum, but misses small gaps in what turn out to be narrow bands in the low field limit \[13\].

**Semiclassical wavefunctions** - Assuming \( \ell_B \) is larger than any other length scale in the problem (weak fields), we may use a gradient expansion for the wavefunctions \[5\],

\[
\tilde{\psi}(k_1, \tilde{k}) \sim \exp \left[ \hat{\ell}_B^2 \tilde{S} - S_0 + \cdots \right].
\]

We again start with uncoupled layers. Defining \( q_y^\pm(k_1) = \Delta_y \pm Q_y(k_1) \), with \( Q_y(k_1) = \sqrt{E_y^2 - (k_1 - \Delta_x)^2} \), and \( \Delta_x = \tilde{k}, \Delta_y = (-)k_0/2 \) for the top (bottom) layer, the lowest non-trivial contribution has the form

\[
\tilde{\psi}_\pm \sim \exp(\hat{\ell}_B \tilde{S}) J_x(k_0)e^{i\phi}.
\]

The (spinor) coefficient of the wavefunction is determined at higher order in \( 1/\hat{\ell}_B^2 \) \[37\], and is not included in our analysis. The set of momenta \( \{(k_\perp, q_y^\pm(k_\perp))\} \) represent contours of constant energy above and below a Dirac point. When \( Q_y(k_1) \) approaches 0, these two curves approach one another, and the semiclassical approximation breaks down. To account for this one employs matching conditions \[38\] at each turning point. These work simultaneously at certain discrete energies, yielding a spectrum with spacing matching the exact result for Landau levels of a single Dirac point Hamiltonian.

This result is essentially correct even in the presence of interlayer tunneling when one considers levels close in energy to that of the Dirac points. For energies near those of the saddle points, one must develop further connection formulae among the different semiclassical trajectories \[5\]. This is most easily implemented for \( \tilde{V}_0 \), which connects trajectories near \( M_s \) in Fig. 1. The cases of \( \tilde{V}_1 \) are somewhat more complicated \[39\]. \( \tilde{V}_1 \) connects the wavefunction for \( \tilde{k} \) in the top layer with that of the bottom layer for \( \tilde{k} - G_x/2 \), via the saddle point \( M_s \), using the operator \( \tau(\hat{G}_1) \). The problem becomes closely analogous to that of the \( M_s \) saddle point if one applies a unitary transformation, shifting the bottom component of the wavefunctions by \( \tau(\hat{G}_1) \). This is represented conveniently by placing one quarter of the BZ for \( \tilde{k} - G_x/2 \) continuously onto the upper right side of the \( \tilde{k} \) BZ. Similar constructions for \( \tilde{V}_1 \), \( \tilde{V}_2 \), and \( \tilde{V}_3 \) bring in another quarter of the \( \tilde{k} - G_x/2 \) BZ on the lower right, and half of the \( \tilde{k} + G_x/2 \) BZ on the left, yielding a doubled BZ in the form of a rectangle. This is illustrated in Fig. 1 along with relevant semiclassical orbits, which are labeled with unprimed (primed) numbers for the \( \tilde{k} \) \( \tilde{k} + G_x/2 \) BZ.

Wavefunctions for the full system involve amplitudes multiplying functions of the form in Eq. 6, with the caveat that \( \Delta \) represents the location of the Dirac point around which an orbit is centered. We assign an amplitude for each trajectory that enters or exits a saddle point, which are related to one another in several ways. (i) Each trajectory has an amplitude \( a_i^\pm \) to exit from some saddle point and an amplitude \( a_i^\pm \) to enter another. These are related by \( a_i^\pm = (1, \pm i)e^{i\Phi_i/\ell_B} \), where \( \Phi_i/\ell_B \) is the area between the trajectory (which begins and ends at the points of closest approach to the saddle points) and the \( q_y = 0 \) axis in Fig. 1. This area is taken to be positive (negative) if the trajectory is above \( k_1 \)-axis and moves to the right (left). Factors of \( \pm i \) must be inserted if there is a left or right turning point in the trajectory \[38\]. (ii) At each saddle point shown in Fig. 1, there are two incoming trajectories and two outgoing ones. These are related by an \( S \)-matrix, which we discuss in more detail below. (iii) Trajectories exiting the doubled BZ on the left or right are related to ones entering on the opposite side due to the periodicity imposed by the MT operators. The effect of this can be incorporated in the matrices relating different amplitudes with some added (energy independent) phase factors \[34\]. In practice, their presence only impacts the spectrum for energies rather close to that of the saddle points.

The \( S \)-matrix associated with the saddle points can be obtained through the two-band model, Eq. 2. Introducing the magnetic field by adding a vector potential to the momentum \( k \), one finds the eigenvalue equation can be reduced to a single component problem in the neighborhood of the saddle point at \( k_1 = w \). With a gauge transformation to Landau gauge, one obtains an eigenvalue equation involving a massive particle in an inverted parabolic potential, \[
\frac{\partial^2}{\partial x^2} + \epsilon + \frac{\Delta x^2}{4} \psi = 0
\]

with \( \epsilon = \frac{\ell_B^2 (E'^2 - w^2)}{2\sqrt{(w - E')/\ell_B}} \) and \( X = \sqrt{3}(k_1 - w)\ell_B \left[ \frac{w - E'}{\Delta x} \right] \). Here we define \( E' = E - k_0/2 \). The resultant \( S \)-matrix
Numerical solutions to the problem described above are illustrated in Fig. 2 and are consistent with direct numerical diagonalization [24] of the Hamiltonian in Eq. (3). Relatively simple behavior is apparent well below and above the saddle point energy, which may be understood analytically. Below the saddle point, interlayer tunneling is negligible, leading to $\hat{Q}_i \to \hat{I}_d$. Moreover, $\sum \gamma A_\gamma = A = \pi E^2$, which is the area enclosed by a trajectory in an uncoupled layer, and $\sum \gamma D_\gamma = 0$. This leads to the standard Dirac-Landau level spacing.

Above the saddle point, one finds $\hat{Q}_a \to i \hat{I}_2 \otimes \hat{\sigma}_x$ and $\hat{Q}_b = \hat{Q}_c \to i \hat{\sigma}_x \otimes \hat{\sigma}_z$. These anticommute with $\hat{\Gamma}$, and one can show that Eq. (8) is satisfied if $e^{i \Gamma_2 (A \pm X)} + i = 0$ for either one of the two signs in the exponent. In this expression, $A = D_{ab} + D_{ca} - D_{bc} = 3 \sqrt{3} k_B E/2$, and $\chi(E = k_B E)$ corresponds to the area of half of a single BZ. The quantities $A + (-) \chi$ are areas related to the star-like orbits, which increase (decrease) in magnitude with energy, leading to coexisting electron- and hole-like levels.

Discussion – The spectrum predicted above resolves some apparent inconsistencies among recent results. Studies which include only one saddle point [22, 23, 42, 43] yield purely electron-like spectra. By contrast, one expects hole-like orbits surrounding local maxima to come down towards the saddle point, as shown in tight-binding studies of the twisted bilayer [25]. These pictures are in a sense both correct. When several SP’s are degenerate in energy, the necessity to include multiple BZ’s allows electron- and hole-like orbits to coexist. Importantly, this structure explains how levels rising from below the SP and levels falling from above with increasing $B$ evolve: the levels anti-cross, and all ultimately move to high energy when the field is sufficiently large, as is evident in Fig. 2. This behavior should appear in many systems where degenerate, distinguishable SP’s allow a transition between topologically distinct semiclassical orbits, including graphene on boron nitride substrates [14, 15], and in single layer graphene at high energy [16]. This behavior is also apparent in the surface states of crystalline topological insulators in a magnetic field [44].

The peculiar Landau level structure and the associated semiclassical orbits in our model should have a number of experimental ramifications. For sufficiently clean samples, the level structure itself could be detected directly in tunneling [7]. Cyclotron resonance [45–47] brings another interesting perspective: since star-like orbits tunnel periodically between layers, electromagnetic waves with electric field perpendicular to the layers should couple to them and allow absorption, whereas in truly two-dimensional systems this would not be possible. (Preliminary calculations [59] demonstrate that this is indeed the case.) Thermodynamically, converging hole-like and electron-like orbits at the saddle point energy should lead to cusp-like behavior in magnetic susceptibility [48]. Finally, breaking the symmetry among the saddle points, for example by strain or a periodic potential [59], can in principle induce open orbits, which might be observed in transport as a metal-insulator transition.

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Supplementary Material

Saddle Point Dispersion from $\vec{k} \cdot \vec{p}$ Approximation

Near $M_a$, the electron wavefunction may be taken as proportional to $e^{i\vec{k} \cdot \vec{r}}$, with small $k = \sqrt{k_1^2 + k_2^2}$, independent of layer index. Only $\hat{V}_0$ is relevant to the spectrum in this small range of momentum, and small terms of order $k$ can be treated perturbatively. The form of $\hat{V}_0$ is simplified by the transformation $\hat{U}^\dagger \hat{t}_0 \hat{U} = \hat{I}_2 + \hat{\sigma}_z$ with $\hat{U} = \exp [-i \frac{\pi}{2} \hat{\sigma}_y]$, and the transformed $\hat{V}_0$ now has only one nonzero matrix element. With the unitary transformation,

$$ B = \begin{pmatrix} \hat{U} & 0 \\ 0 & \hat{U} \end{pmatrix} \times \begin{pmatrix} 1 \\ \hat{\sigma}_x \end{pmatrix},$$

(9)

in which the latter matrix exchanges the second and third rows and columns, we may transform the Hamiltonian into

$$ \hat{H}_{sp} = B^\dagger \hat{H} B = \begin{pmatrix} 2w \hat{\sigma}_x & ik_2 \hat{\sigma}_z \\ -ik_2 \hat{\sigma}_z & 0 \end{pmatrix} + \begin{pmatrix} k_1 \hat{1}_2 & -ik_2 \hat{\sigma}_z \\ ik_2 \hat{\sigma}_z & -k_1 \hat{1}_2 \end{pmatrix}. $$

(10)

It is easy to diagonalize the first matrix, $\hat{H}_0$, and the its four eigenvalues are given by

$$ \lambda_{1,2}^+ = -\lambda_{1,2}^- = \pm \sqrt{\frac{k_0^2 + 4w^2}{2}},$$

(11)

where $w$ is positive and we assume $\lambda_1^+ > \lambda_2^+$, $\lambda_1^- = -\lambda_2^-$. Defining ket vectors in terms of eigenstates of $\hat{\sigma}_x$, $\sigma_x | \pm > = \pm | \pm >$ and the constant $\beta = \sqrt{\lambda_2^+ / \lambda_1^+}$, the normalized eigenvectors are given by

$$ |\lambda_1^+ \rangle = \frac{1}{\sqrt{2 - 4\alpha}} \left( |+ > -i\beta | - > \right),$$

(12)

and

$$ |\lambda_2^+ \rangle = \frac{1}{\sqrt{2 + 4\alpha}} \left( | - > - i\beta^{-1} | + > \right),$$

(13)

for the positive energy eigenstates. Note that $\beta^2 = 1 - 4\alpha$. Their negative energy counterparts are

$$ |\lambda_1^- \rangle = \frac{1}{\sqrt{2 - 4\alpha}} \left( | - > + i\beta | + > \right),$$

(14)

and

$$ |\lambda_2^- \rangle = \frac{1}{\sqrt{2 + 4\alpha}} \left( |+ > + i\beta^{-1} | - > \right).$$

(15)

Because $\lambda_i^+ = -\lambda_i^-$ for $i = 1, 2$, there is an antiunitary relation between the states of the form

$$ |\lambda_i^+ \rangle = [\hat{t}_3 \otimes \sigma_3] K |\lambda_i^- \rangle, \ i = 1, 2.$$  

(16)

in which complex conjugation is represented by $K$.

The perturbation in $k_1$ and $k_2$, the second term in Eq. 10 may be expressed as

$$ H_1 = k_1 [\hat{\sigma}_3 \otimes \hat{1}_2] + k_2 [\hat{\sigma}_2 \otimes \hat{1}_2],$$

(17)
with which one may verify the matrix elements

\[
< \lambda^+_1 | H_1 | \lambda^+_1 > = - < \lambda^+_2 | H_1 | \lambda^+_2 > = 2 \alpha k_1 .
\]  

(18)

These diagonal matrix elements contain no contribution from \( k_2 \). On the other hand, \( k_2 \) does appear in the off-diagonal matrix element,

\[
< \lambda^+_1 | H_1 | \lambda^-_2 > = - k_2 .
\]

(19)

These matrix elements define an approximate projection of \( H_1 \) into the positive eigenvalue subspace of the \( k = 0 \) Hamiltonian in Eq. 10. A correction to this can be included in the diagonal elements in Eq. (18) using second-order perturbation theory, with the negative energy states, Eqs. 14 and 15, being the intermediate states. Using

\[
< \lambda^+_1 | H_1 | \lambda^-_1 > = 0, \quad < \lambda^+_1 | H_1 | \lambda^-_2 > = k_1
\]

(20)

and

\[
< \lambda^+_2 | H_1 | \lambda^-_1 > = 0, \quad < \lambda^+_2 | H_1 | \lambda^-_2 > = k_1
\]

(21)

the correction to the both diagonal terms is the same, with

\[
\frac{|< \lambda^+_1 | H_1 | \lambda^-_2 >|^2}{\lambda^+_1 - \lambda^-_2} = \frac{|< \lambda^+_2 | H_1 | \lambda^-_1 >|^2}{\lambda^+_2 - \lambda^-_1} = \frac{k_1^2}{k_\theta} .
\]

(22)

Putting these results together, the projection of \( H_1 \) onto the states \( \{ | \lambda^+_1 > \} \) can be expressed approximately as a two-band Hamiltonian,

\[
H_1 \mapsto \frac{k_1^2}{k_\theta} \hat{I}_2 + 2 \alpha k_1 \hat{\sigma}_z - k_2 \hat{\sigma}_x .
\]

(23)

Together with the unperturbed Hamiltonian \( H_0 \mapsto \frac{\lambda^+_1 + \lambda^+_2}{2} \hat{I}_2 + \frac{\lambda^+_1 - \lambda^-_1}{2} \hat{\sigma}_3 \), the two-band Hamiltonian in the main text (Eq. 2) is obtained.

**Saddle Point Hamiltonian from Two Band Model**

For the purpose of computing the \( S \)-matrix, we may choose any convenient gauge. The wavefunctions well away from the saddle point have distinct in-coming and out-going characters on either side of it, so that a gauge transformation does not affect the \( S \)-matrix itself. To compute the \( S \)-matrix we adopt Landau gauge, so that introducing the vector potential can be implemented via the substitution \( k_2 \rightarrow k_2 - \frac{i}{\ell_B} \partial_{k_1} \), while \( k_1 \) remains unchanged. The energy reference is set by \( E' = E - k_\theta / 2 = 0 \). The corresponding equations for the two-band model become

\[
(V_A - E')u + \frac{i}{\ell_B} \frac{\partial_{k_1} u}{\partial k_1} = 0 ,
\]

(24)

\[
\frac{i}{\ell_B} \frac{\partial_{k_1} u}{\partial k_1} + (V_B - E')v = 0 ,
\]

(25)

where

\[
V_{A(B)}(k_1) = \frac{(k_1 \pm w)^2}{k_\theta} \pm (1 \mp \alpha)w .
\]

(26)
One may eliminate the $u$ term to arrive at

$$\frac{1}{\ell_B} V_A' u' - (V_A - E')(V_B - E') v - \frac{1}{\ell_B^2} \partial^2 \partial k^2 v = 0,$$

and furthermore eliminate the derivative term $v'$ by writing $v = \sqrt{V_A - E'} \psi$ to obtain

$$- \frac{1}{\ell_B} \psi'' + (E' - V_A)(V_B - E') \psi = 0 + O(\ell_B^{-4}).$$

For the band containing the saddle point, $E' < 0$. The factor $(V_A - E')(V_B - E')$ on the left-hand side of the above equation in this situation has the form of an inverted parabola in the neighborhood of $k_1 = w$, which can be approximated as

$$(V_A - E')(V_B - E') \approx [E' - (1 + 3\alpha)w] \left[ \frac{(k_1 - w)^2}{k_\theta} - w(1 + \alpha) - E' \right].$$

Then we may then rewrite Eq. (28) in the form

$$\left[ \frac{d^2}{dX^2} + \frac{X^2}{4} + \epsilon \right] \psi = 0,$$

with

$$X = \sqrt{2}\ell_B(k_1 - w) \left[ \frac{(1 + 3\alpha)w - E'}{k_\theta} \right]^{1/4}$$

and

$$\epsilon = \sqrt{k_\theta \ell_B} \frac{[E' + (1 + \alpha)w][E' - (1 + 3\alpha)w]}{2\sqrt{(1 + 3\alpha)w - E'}}.$$  

From this expression one may compute the $S$-matrix using standard methods as described in the text. Incoming and outgoing states on either side of $X = 0$ correspond to such states for the original Hamiltonian, and this same $S$-matrix connects the amplitudes for those states. The expressions for $X$ and $\epsilon$ in the main text are obtained by setting $\alpha = 0$ for the purpose of simplifying the expressions; the actual numerical computation still uses the expressions listed here.
Derivation of Equation 8

The incoming and outgoing amplitudes near saddle points $M_a$ and $M'_a$ are related through,

\[
\begin{pmatrix}
2 \\
4 \\
2' \\
4'
\end{pmatrix} = \begin{pmatrix}
S_0 & 0 \\
0 & U_\phi S_0 V_\phi
\end{pmatrix} \begin{pmatrix}
1 \\
6 \\
1' \\
6'
\end{pmatrix}_o \equiv Q_a \begin{pmatrix}
1 \\
6 \\
1' \\
6'
\end{pmatrix}_o,
\]

in which the parameter $\phi$ encodes the boundary condition between the edges of the doubled BZ, and the basic $S$-matrix $S_0$ is given in the main text. The 2x2 unitary matrices,

\[
U_\chi \equiv \begin{pmatrix}
1 & 0 \\
0 & e^{i\chi}
\end{pmatrix}, \quad V_\chi \equiv \begin{pmatrix}
e^{i\chi} & 0 \\
0 & 1
\end{pmatrix},
\]

specify the boundary conditions.

The subsequent phase accumulation between saddle points $M_a$ and $M'_b$ (arc 1 and 6 in first BZ) and that between $M'_a$ and $M_b$ (arc 1' and 6' in the second BZ) is represented by

\[
\begin{pmatrix}
1 \\
6 \\
1' \\
6'
\end{pmatrix} \equiv e^{-iA_{ab} + iD_{ab}} \hat{\Gamma} \begin{pmatrix}
1 \\
6 \\
1' \\
6'
\end{pmatrix}_o \equiv R_{ab} \begin{pmatrix}
1 \\
6 \\
1' \\
6'
\end{pmatrix}_o,
\]

in which $\hat{\Gamma} = \hat{\sigma}_z \otimes \hat{I}_2$. The quantities $A_{ab}$ and $D_{ab}$ appearing in the exponent combine to give the areas between the numbered arcs and the $k_1$ axis. We shall represent these areas in terms of the five elementary areas $a - e$ defined in Fig. 3. Before we proceed to show how the representation of area is done, one should notice that arcs 1 and 6 (see Fig. 1 in the main text) in first BZ should sweep out identical areas since the orbits are symmetric about the $k_1$ axis and move in opposite directions. The same is true for arcs 1' and 6' in the second BZ. One may show that

\[-(A_{ab} - D_{ab}) = a + \frac{b - d}{2}\]

is the shading area associated with arc 1 in the top-left of Fig. 3. It can be seen that $(-a)$ is the negative (brown) area contributed from the left side of circle, and $(d - b)/2$ is the positive (green) shaded area. Similarly, one may show that the area associated with arc 6' is

\[-(A_{ab} + D_{ab}) = a + \frac{b + c + e}{2}.\]

Note that the overall minus sign is due to the choice of circulation of those closed trajectories specified by the arrow in Fig. 3. Continuing the same procedure, one can write down the relations at the saddle point $M_b$ and $M'_b$,

\[
\begin{pmatrix}
1 \\
6 \\
1' \\
6'
\end{pmatrix}_o = \hat{Y} \begin{pmatrix}
U_\theta S_0 U_\theta^\dagger \\
0 \\
V_\theta^\dagger S_0 V_\theta
\end{pmatrix} \hat{Y} \begin{pmatrix}
3 \\
5 \\
3' \\
5'
\end{pmatrix}_o \equiv Q_b \begin{pmatrix}
3 \\
5 \\
3' \\
5'
\end{pmatrix}_o,
\]

with

\[
\hat{Y} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix}.
\]
The reordering matrix $\hat{Y}$ implements the property that the $M_b$ and $M'_b$ SP’s scatter trajectories between different BZ’s. $\theta$ is another phase angle parameter encoding the eigenvalues under the MT operators. The next phase accumulation is given by

$$
\begin{pmatrix}
3 \\
5 \\
3' \\
5'
\end{pmatrix}_{o} = e^{-iA_{bc}e^{iD_{bc}}}\begin{pmatrix}
1 & 0 \\
0 & V_\phi U_\phi^\dagger
\end{pmatrix}\begin{pmatrix}
3 \\
5 \\
3' \\
5'
\end{pmatrix}_{o} \equiv R_{bc} \begin{pmatrix}
3 \\
5 \\
3' \\
5'
\end{pmatrix}_{o},
$$

(38)

with the area

$$-(A_{bc} - D_{bc}) = b + c + d$$

specifying the phase along arcs 3 and 5 (top-right in Fig. 3), and

$$-(A_{bc} + D_{bc}) = b - e$$

specifying the phase along arcs 3' and 5' (bottom-right in Fig. 3). Finally, the scattering at $M_c$ and $M'_c$ may be written as

$$
\begin{pmatrix}
3 \\
5 \\
3' \\
5'
\end{pmatrix}_{o} = Y \begin{pmatrix}
V_\phi^\dagger S V_\phi & 0 \\
0 & U_\phi S U_\phi^\dagger
\end{pmatrix} Y \begin{pmatrix}
2 \\
4 \\
2' \\
4'
\end{pmatrix}_{o} \equiv Q_c \begin{pmatrix}
2 \\
4 \\
2' \\
4'
\end{pmatrix}_{o},
$$

(39)

and the subsequent phase accumulation by

$$
\begin{pmatrix}
2 \\
4' \\
2' \\
4'
\end{pmatrix}_{o} = e^{-iA_{ca}e^{iD_{ca}}}\begin{pmatrix}
2 \\
4' \\
2' \\
4'
\end{pmatrix}_{o} \equiv R_{ca} \begin{pmatrix}
2 \\
4' \\
2' \\
4'
\end{pmatrix}_{o}.
$$

(40)

The corresponding areas for arcs 2 and 4 are the same as those for arcs 1 and 6, and arcs 2' and 4' are the same as for arcs 1' and 6'. Putting together Eqs. 33, 35, 36, 38, 39 and 40 leads to Eq. 8 in the main text.

Finally, for the next section it is useful to note the relations

$$A_{ab} + A_{bc} + A_{ca} \equiv A = 2a + 2b + c. \quad (41)$$

For energies below that of the saddle point, one finds (excluding corrections of order $\alpha$) $A = \pi E^2$, which corresponds to the circular area associated with the trajectories of energy below that of the saddle point. Moreover,

$$D_{ab} + D_{bc} + D_{ca} = 0, \quad D_{ab} - D_{bc} + D_{ab} = -(c + d + e) \equiv -X. \quad (42)$$

Again excluding corrections of order $\alpha$, one finds $X = 3\sqrt{3}k\theta E/2$. This is relevant for the quantization condition above the saddle point.

**Energy Level Conditions Above/Below Saddle Point**

For energy sufficiently below the saddle point, $E' \ll -w$, the basic S-matrix reduces to $S_0 \rightarrow \hat{I}_2$, which leads to all $Q$’s equal identity matrix as well. Because the sum of $D$’s vanishes and the sum of $A$’s equals the Dirac circle area, it is easy to show that Eq. 8 in the text reduces to

$$e^{i\ell_2 A} = 1, \quad (43)$$
\begin{table}
\centering
\begin{tabular}{|c|c|}
\hline
arc number & area \\
\hline
1,2 & \(- (a + \frac{b}{2}) + \frac{d}{2}\) \\
4,6 & \(- (a + \frac{b}{2}) + \frac{d}{2}\) \\
1',2' & \(- (a + \frac{b+c+d}{2})\) \\
4',6' & \(- (a + \frac{b+c+d}{2})\) \\
3,5 & \(- (b + c + d)\) \\
3',5' & \(- b + e\) \\
\hline
\end{tabular}
\caption{Representation of the area between the portions of trajectories (See Fig. 1 in main text for numbering) and \(k_1\) axis using the five elementary areas shown in Fig.3 of the supplement. The pair of numbered arcs appearing in the same row correspond to the same area due to the orbit symmetry with respect to \(k_1\) axis and the fact that they move in opposite directions. Arcs 1, 3, 6', and 5' are four representative orbits for demonstrating the areas in terms of the elementary ones \(a - e\) in Fig.3.}
\end{table}

which gives the ordinary Landau levels for single layer graphene.

For energy sufficiently above that at the saddle point, the \(S_0 \mapsto i\hat{\sigma}_1\). For simplicity, we set \(\theta = \phi = 0\). The product of the six matrices \(Q_a \hat{R}_{ab} Q_b \hat{R}_{bc} Q_c \hat{R}_{ca}\) can be written as

\[
(i)^3 e^{iA} \left[ \hat{1}_2 \otimes \hat{\sigma}_x \right] e^{-i \frac{i}{2} \hat{\Gamma}} [\hat{\sigma}_x \otimes \hat{\sigma}_x] e^{i \frac{i}{2} \hat{\Gamma}} [\hat{\sigma}_x \otimes \hat{\sigma}_x] e^{-i \frac{i}{2} \hat{\Gamma}} = (-i)e^{iA} \left[ \hat{1}_2 \otimes \hat{\sigma}_x \right] e^{-i \hat{\Gamma}},
\]

where we have written \(D_{ab} = D_{ca} = -2D_{bc} = -\chi/4\). We have also used the facts that \(\hat{\sigma}_x \otimes \hat{\sigma}_x\) in the brackets anticommutes with \(\hat{\Gamma} = \hat{\sigma}_z \otimes \hat{1}_2\), that its square is the unit matrix . Eq. 8 in the text then reduces to

\[
\det \begin{pmatrix}
 e^{i\alpha} + ie^{-i\chi} \hat{\sigma}_x & 0 \\
 0 & e^{i\alpha} + ie^{i\chi} \hat{\sigma}_x
\end{pmatrix} = 0.
\]

which leads to two possible conditions for the allowed areas,

\[
\cos \left[ \ell_B^2 (\alpha \pm \chi) \right] = 0.
\]

Note that we have set \(\ell_B^2 = 1\) in all expressions in this Supplement except the last one. The inclusion of boundary conditions specified by \(\theta\) and \(\phi\) can be shown to yield identical spectra away from the saddle point. However, for energies close to the saddle point, the magnetic states are indeed altered by these parameters. This is illustrated in Fig. 4 below, which show how the states in a range of energies behave for various values of \((\theta, \phi)\).
FIG. 3: (Color online) Representation of $A$’s and $D$’s in Eqs. 35, 38 and 40 by the shaded areas associated with the representative arcs. Circles in top row are the trajectories of top layer in first BZ, while those in bottom row are for the trajectories of bottom layer in second BZ (See Fig. 1 in main text). Because the orbits are symmetric about the $k_1$ axis, arc 1 in top-left is the representative of arcs $\{1, 2, 4, 6\}$ all of which under the specified circulation correspond to the same area listed in Table I. Similarly, arc 3 on top-right, arc 6' on bottom left, and arc 5' on bottom right are the representative ones. The five elementary areas $a$ -- $e$ specified by either shape or color are listed in the right column. Referring to the circle in bottom-right, the circle of area $\pi r^2$ with $r = E$ is divided into three distinct parts, the gold box in the middle of area $c$, the side of area $a$ and the top/bottom portion of area $b$. The green box of area $d$ in top-right and the purple box of area $e$ in bottom-right are different because the Dirac points (the center of circle) in top and bottom rows have different distances, $h = k_0/2$ and $2h$, respectively, from the $k_1$ axis.

FIG. 4: Detailed views of the states near the saddle point for various boundary conditions specified by the parameters $\theta$ and $\phi$. The spectrum away from saddle point at $E' = -0.05$ does not change with these parameters.