WKB estimate of bilayer graphene’s magic twist angles

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Graphene bilayers exhibit zero-energy flat bands at a discrete series of magic twist angles. In the absence of intra-sublattice inter-layer hopping, zero-energy states satisfy a Dirac equation with a non-abelian SU(2) gauge potential that cannot be diagonalized globally. We develop a semiclassical WKB approximation scheme for this Dirac equation by introducing a dimensionless Planck’s constant proportional to the twist angle, solving the linearized Dirac equation around AB and BA turning points, and connecting Airy function solutions via bulk WKB wavefunctions. We find zero energy solutions at a discrete set of values of the dimensionless Planck’s constant, which we obtain analytically. Our analytic flat band twist angles correspond closely to those determined numerically in previous work.

Introduction —. At a discrete set of magic twist angles, bilayer graphene develops low-energy flat bands [1, 2] that lead to strong correlation physics including surprising superconductivity [3, 4], novel orbital magnetism [5–8], and the quantum anomalous Hall effect [9–11]. The presence of narrow bands has recently been attributed to a twist-angle-dependent non-abelian SU(2) gauge field in bilayer graphene [2, 15–17]. In the case of 2D Dirac fermions with a magnetic field represented by an abelian U(1) gauge field, it has long been known that robust zero-energy states appear at any magnetic field strength [13–21], with degeneracy equal to the total number of flux quanta [22, 23]. In this work we explain why flat bands emerge only at quantized field strengths, corresponding to almost equally spaced inverse twist angles [2], in the SU(2) case.

Our analysis is based on a WKB-like approximation in which we define a dimensionless effective Plank’s constant $\beta$ that is proportional to twist angle. The WKB approximation breaks down near the high-symmetry AB and BA stacking points in each unit cell of the twisted bilayer moiré pattern. Linearizing the Dirac equation around these turning points leads to Airy function local solutions. By connecting the Airy functions in their asymptotic regions to the WKB solutions, we derive a connection formula that glues the local solutions together to form a global wave function. Because of a topological obstruction, the approximate global solution is well defined only at discrete $\beta$ values whose inverses are equally spaced. The set of twist angles that are defined by this condition agrees closely with those identified numerically in the previous work [2].

Model —. We study the chiral symmetric model of twisted bilayer graphene [2, 16], whose Dirac Hamiltonian $H = v_D (p + \alpha A) \cdot \sigma$ describes 2D Dirac fermions with velocity $v_D$, in the presence of a non-dynamical SU(2) gauge field $A$ that acts on the layer degree of freedom. The gauge potential $A = (A_x, A_y) = (\sum_i A_{x,i} \tau_i, \sum_i A_{y,i} \tau_i)$ arises physically from local-stacking-dependent interlayer tunneling and is a periodic function of position in the twisted bilayer. Here $\sigma$ and $\tau$ are respectively sublattice and layer Pauli matrices. The non-abelian nature of this equation arises from the nonzero commutator of $A_x$ and $A_y$. The two gauge potential components cannot be diagonalized simultaneously, and the equation therefore cannot be reduced to its well-understood abelian counterpart.

In this Letter we focus on zero energy solutions. Following Ref. 2 we take advantage of chiral symmetry to simplify the analysis by expressing the Hamiltonian as $H = \alpha D \sigma_- + \alpha D^\dagger \sigma_+$ with $\sigma_\pm = (\sigma_x \pm i \sigma_y)/2$ and $D = (p_x + ip_y)/\alpha + A_x + i A_y$. It follows that zero energy solutions appear in pairs that are polarized on different sublattices. One of the solutions satisfies $\mathcal{D} \psi = 0$, or more explicitly upon inserting the explicit form of the interlayer tunneling Hamiltonian [2]

$$\begin{pmatrix} -2i\beta \hat{D} & U(r) \\ U(-r) & -2i\beta \hat{D} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0,$$

where the two components are amplitudes in different layers, $\beta = \hbar/\alpha$ acts as an effective Plank’s constant, $U(r) = \sum_j e^{i j \beta r} q_j e^{-iq_j r}$ is complex, and $\phi = 2\pi/3$. The $q_j$ ($j = 1-3$) are equivalent moiré Brillouin zone corner wavevectors whose common magnitude $k_\theta = 2k_\theta / \sin(\theta/2)$, where $k_\theta$ is the graphene Brillouin zone corner wavevector magnitude, is inversely proportional to twist angle $\theta$ for small twists. $U(r)$ has the translational periodicity of the moiré pattern. Since the dimensionless coupling constant $\alpha$ in the Dirac equation is $\alpha = t_\perp / h v_D k_\theta$ where $t_\perp \sim 100$ meV is the interlayer tunneling strength, $\beta$ is proportional to twist angle and vanishes in the small twist angle semiclassical limit. Below we set $\hbar \rightarrow 1$ and measure momenta and positions in units of $k_\theta$ and $k_\theta^{-1}$.

WKB approximation —. Following the WKB approach we seek solutions of Eq. (1) that are linear combinations of $e^{i S/\beta}$ and $e^{-i S/\beta}$. Expanding $S$ in powers of $\beta$ and truncating at leading order yields the two-parameter ap-
proximate form (valid for either $\psi_1$ or $\psi_2$)

$$
\psi = \frac{C_+}{\sqrt{A}} \left[ -\frac{U(\vec{r})}{\sqrt{U(-\vec{r})}} \right] e^{iS/\beta} + \frac{C_-}{\sqrt{A}} \left[ \frac{\sqrt{U(\vec{r})}}{\sqrt{U(-\vec{r})}} \right] e^{-iS/\beta}.
$$

where

$$
\partial S = A/2 \tag{3}
$$

and $A(\vec{r}) = \sqrt{U(\vec{r})U(-\vec{r})}$ is a local wavevector related to the gauge potentials $U(\pm \vec{r})$. Eq. (3) can be solved by employing a Fourier transform method that rewrites

$$
A = \sum_{\vec{G}} A_{\vec{G}} e^{i \vec{G} \cdot \vec{r}} = \sum_{\vec{G}} A_{\vec{G}} e^{i \left( \vec{G} \cdot \vec{r} + \vec{G} \cdot \vec{z} \right)}
$$

where $A_{\vec{G}}$ is a Fourier coefficient, $\vec{G} = (G_x, G_y)$ is a moiré reciprocal lattice vector, $G = G_x + iG_y$, and $\vec{G} = G_x - iG_y$. Using the Fourier expansion for $A$ in Eq. (3) and integrating yields

$$
S = S^c(\vec{z}) + \frac{1}{2} A_0 \vec{z} \cdot \vec{z} + \sum_{\vec{G} \neq 0} \frac{1}{iG} A_{\vec{G}} e^{i \left( \vec{G} \cdot \vec{z} + \vec{G} \cdot \vec{z} \right)} \tag{4}
$$

where the last term is related to the periodic spatial variation of $A$, and the second term to its spatial average. The first term $S^c(\vec{z})$ is an arbitrary function of $\vec{z}$. Requiring the imaginary part of $S$ (the log of the magnitude of the wavefunction) to be bounded fixes $S^c(\vec{z}) = A_0 \vec{z}/2$, up to a constant.

In Fig. 1, we illustrate the dependence of $A$, which is defined only up to a sign, on position within one moiré unit cell by representing its real and imaginary parts by the horizontal and vertical components of $\vec{A} = (\text{Re}A, \text{Im}A)$. This vector and its negative are the Dirac points of the local band structure calculated at a given position $\vec{r}_0$ by setting $A(\vec{r})$ to its value at $\vec{r} = \vec{r}_0$. Eq. (3) states that the complex derivative of $S$ with respect to $\vec{z}$ is equal to the complex momentum $A_x + iA_y$ at each position. In Figs. 2(a) and 2(b), the corresponding real and imaginary parts of $S$ are plotted separately. Importantly both real and imaginary parts of $S$ are nonzero, unlike the one-dimensional WKB case in which $S$ is imaginary in the classically forbidden regions and real in the classically allowed region. By performing the derivative with respect to $z$ on both sides of Eq. (4), we find that in the present case $\nabla^2 \text{Im}S = (\partial_x \text{Im}A - \partial_y \text{Re}A)$; the curl of the vector $\vec{A}$ depicted in Fig. 1 which is non-zero, behaves like a source for $\text{Im}S$: Similarly, $\nabla^2 \text{Re}S = \nabla \cdot \vec{A}$, implying that $\nabla \text{Re}S$ is equal to the local wavevector up to divergence-free function.

**Turning points and Stokes lines**. $A$ has a simple zero at the AA stacking point in the moiré cell, and square root singularities at both AB and BA points. The square root singularities introduce a branch cut that lies along the wavy purple lines in Fig. 1 when we choose the real part of $A$ to be non-negative; it is not possible to choose $A$ to be both smooth and single-valued. The two branches as a set change continuously, however, since $A$ connects smoothly to $-A$ across these lines. When $|A| \gg \beta$ either branch of $A$ provides an accurate local solution to Eq. (1). Three Stokes lines can be identified that radiate from AA to AB and BA stacking points as indicated by the dotted lines in Fig. 2 and the purple dotted lines in Fig. 3. We define the Stokes lines by the condition that $\vec{A} \cdot d\vec{l} = \text{Re}A \vec{z} \cdot d\vec{l} = 0$, following the definition used in the well studied case $24, 25$ where $A$ and $S$ are analytical functions that depend only on $\vec{z}$. The Stokes lines form a network that divides the two-dimensional plane into domains distinguished in Fig. 3 by Roman numerals I-VI. In the analytic case $24, 25$ the WKB solution coefficients $C_{\pm}$ change across the Stokes lines because the real part of $S$ is constant and the wavefunction stops oscillating.
Since $\text{Re}A$ is nearly constant along the Stokes line in our case (see Fig. 2a) we will assume that we can also allow different coefficients in regions that are separated by Stokes lines. The WKB solutions are piecewise well-defined inside each domain away from turning points and Stokes lines. To connect the WKB solutions in different domains, we need to obtain the local wavefunctions near the turning points that bridge the isolated domains.

Near the AB and BA turning points, $A$ vanishes, the WKB wavefunctions in Eq. (2) are singular, and the WKB approximation is invalid. A good approximation to the wavefunctions near the turning points which is free from singularities can be obtained by linearizing the gauge potential. Near the AB points for example, $U(r) \simeq -\frac{1}{4} e^{i\phi}(\bar{z} - \bar{z}_+)$, where $\bar{z}_+$ is the value of the $\bar{z}$ coordinate at the AB point and $U(-r) \simeq 3e^{-i\phi}$. Note that the linearized gauge potential depends only on the complex coordinate $\bar{z}$. Substituting the expansion in Eq. (1), we obtain the general solution

$$\psi_2 = C_A Ai(\bar{z}') + C_B Bi(\bar{z}')$$

$$\psi_1 = i2\partial\psi_2/3e^{-i\phi}$$

where $\bar{z}' = c(\bar{z} - \bar{z}_+)$ with $c = [9/(8\beta^2)]^{1/3}$, and $C_{A,B}$ are the undetermined coefficients for Airy functions $Ai$ and $Bi$. It is noteworthy that both Airy functions are retained here, in contrast to the one-dimensional WKB analysis. In the one-dimensional confinement potential problems, the wavefunction is required to decay exponentially as the coordinate goes to infinity. The asymptotic behavior of $Bi$ increases exponentially and thus is discarded. Here, the solutions are confined to a finite regime in the complex plane and both functions can contribute to the solution.

**Connection formula**. Although the WKB and Airy function solutions are obtained independently as good local approximations, there are regions, schematically indicated by the area between the solid and dashed circles in Fig. 4, where both approximations are accurate. Inside the dashed circle centered at $\bar{z}_0$ $(1 \gg |\bar{z} - \bar{z}_0|)$, the linearization is justified with whereas, outside the solid circle $(|\bar{z} - \bar{z}_0| \gg (8/9)^{1/3} \beta^{2/3})$, the WKB approximation is reliable and the Airy functions take their asymptotic form. One can therefore make a connection between the WKB and Airy function solutions by comparing them in the overlap region.

We consider the Airy functions solved at point 1 and the WKB solutions in region I in Fig. 3 to illustrate the connection formula derivations. In the region with $|\bar{z}'| \gg 1$, Eq. (5) can be approximated by

$$\psi_2 \simeq (C_A\gamma_{A+} + C_B\gamma_{B+})\bar{z}'^{-1/4}e^{-\beta \bar{z}'^{3/2}} + (C_A\gamma_{A-} + C_B\gamma_{B-})\bar{z}'^{-1/4}e^{\beta \bar{z}'^{3/2}}$$

where $\gamma_{A,\pm}$ and $\gamma_{B,\pm}$ are asymptotic expansion coefficients for $Ai$ and $Bi$, which are different in different regions according to the argument of $\bar{z}'$ separated by the Stokes lines as detailed shown in Supplemental Materials. Specifically, for the region connecting region I to point 1 studied here, $\gamma_{A,+} = -i/2\sqrt{\pi}$, $\gamma_{A,-} = 1/2\sqrt{\pi}$ while $\gamma_{B,+} = 1/2\sqrt{\pi}$ and $\gamma_{B,-} = -i/2\sqrt{\pi}$.

In the same asymptotic region where the WKB approximation also works, one can obtain alternatively the local solution of $S$ by substituting the linearized $U(\pm r)$ into Eq. (3). We find that around the AB point, $S(\bar{z}_+, \bar{z}) = i(\bar{z} - \bar{z}_+)^{3/2}/\sqrt{2} + S_1$ where the first term satisfies the differential equation and $S_1$ is a constant equal to the value of $S$ at turning point 1 obtained by the Fourier transform method. By comparing the WKB and Airy solutions, we find that the exponents $(\frac{3}{5}\beta^{3/2} = (\bar{z} - \bar{z}_+)^{3/2}/\sqrt{2})$ and

![FIG. 3. Stokes diagram in a moiré unit cell bounded by the red solid lines. The red, green, and yellow circles are turning points with local AA, AB, and BA stacking order. The branch cuts and Stokes lines are plotted by purple wavy and dotted lines, respectively. Turning points at the corners are labeled 1-6 while the bounded WKB solution regions are labeled by Roman numerals I-VI.](image1)

![FIG. 4. Validity regions of different solutions in a moiré unit cell. The black regions of different solutions in a moiré unit cell. The black diamond indicates a moiré unit cell with red dots being AA stacking point, yellow and green dots being BA and AB stacking points. The WKB solutions are valid away from the turning points AA, AB, and BA as indicated by the regions outside the black circles in solid lines. The solutions of the linearized equation are valid inside the dashed circle.](image2)
prefactors \((z^{-1/4} = C_{\text{con}}(\bar{z} - \bar{z}_+)^{-1/4}\) with \(C_{\text{con}} = e^{-1/4}\) agree. It follows that the Airy functions and WKB solutions are consistent when the coefficients satisfy
\[
\begin{bmatrix}
C_- \\
C_+
\end{bmatrix}_1 = M_{1,1} \begin{bmatrix}
C_A \\
C_B
\end{bmatrix}_1
\tag{7}
\]
where
\[
M_{1,1} = \frac{1}{C_0 C_{\text{con}}} \begin{bmatrix}
e^{-iS_1/\beta} & e^{-iS_1/\beta} \\
\gamma_{A+} & \gamma_{B+}
\end{bmatrix}
\gamma_{A-} & \gamma_{B-}
\end{bmatrix}
\]
and \(S_1\) is the value of \(S\) at point 1.

Near point 2 in Fig. 3 which is a BA stacking point with complex coordinate \(\bar{z}_-\), we find that \(U(\bar{r}) \simeq \frac{1}{\pi} e^{-i\alpha_2} (\bar{z} - \bar{z}_-)\) and \(U(r) \simeq 3e^{i\alpha_0}\). By redefining the variable \(z = -\bar{z}\) and substituting them into Eq. (11), we can obtain the local solution of \(\psi\) at point 2 as well as its Airy function expansion coefficients at \(\frac{\pi}{\beta}\).

Using their mutual relationships to \(C_{\pm}\) in region I, we see that \(C_{A,B}\) at points 2 and 1 are related
\[
\begin{bmatrix}
C_A \\
C_B
\end{bmatrix}_1 = i \begin{bmatrix}
-a_{1,1} & -a_{1,R} \\
-a_{1,R} & -a_{1,1}
\end{bmatrix} \begin{bmatrix}
C_A \\
C_B
\end{bmatrix}_2
\tag{8}
\]
where \(a_1 = e^{-i(S_1 - S_2)/\beta}\), where \(S_2\) is the value of \(S\) at point 2, and \(a_{1,R}\) stands for the imaginary/real parts.

Similarly, we can obtain the connection formulas for the coefficients of Airy functions at the other neighboring turning points:
\[
T_{12} = i \begin{bmatrix}
-a_{1,1} & -a_{1,R} \\
-a_{1,R} & -a_{1,1}
\end{bmatrix}; T_{23} = \begin{bmatrix}
0 & -2ia_{2,R} \\
0 & -a_{2}
\end{bmatrix}
\tag{9}
\]
where \(a_2 = e^{-i(S_2 - S_3)/\beta}\) depends on the differences of the values of \(S\) at points 2 and 3, and \(a_2\) is its complex conjugate. The phases between other neighboring turning points are the same as either \(a_{1,2}\) or the conjugate of \(a_{1,2}\), as guaranteed by the mirror symmetry of \(A\) in our convention. This symmetry also means that the differences \(S_2 - S_3\) and \(S_1 - S_2\) are real as detailed below.

By setting the cut line at \(y = 0\), we find that the mirror symmetry indicates that the real and imaginary parts of \(A\), i.e., \(Re A\) and \(Im A\), are separately even and odd function of \(y\). Thus, \((\partial_y Im A - \partial_x Re A)/2 = Im(\partial_x A)\) is odd about \(y = 0\), which suggests that \(Im(\partial^2 S) = \frac{1}{\beta^2} Im S\) is also odd following Eq. (13). As a result, up to a constant, \(Im S\) is an odd function about the branch cut, on which \(Im S = 0\) as shown in Fig. (2b).

Therefore, \(S_i - S_j\) is real when points \(i, j\) are on the branch cut and since the amplitudes of \(a_{1,2}\) is \(1\) equal \(1\) one, the determinants of all the matrices above equal \(1\).

**Quantization condition**. The connection formula explained above can glue local solutions together forming a global approximation, which however has a topological obstruction. Specifically, by multiplying the connection formula \(T_{12}T_{23}T_{34}T_{45}T_{56}T_{61}\), one can relate the \(C_{A,B}\) at point 1 to itself. Single-valuedness of the global wavefunction requires that the product of these six matrices have at least one unit eigenvalue. The determinant condition guarantees that unit eigenvalues occur in pairs. Similarly, one can also connect the coefficients at point 2 to itself through \(T_{23}T_{34}T_{45}T_{56}T_{61}T_{12}\) and the same condition is required. The two conditions are not satisfied simultaneously for arbitrary \(\beta\), making the global wavefunction ill-defined. The obstruction disappears at \(\beta\) values for which \(a_{2,R} = 0\), i.e., \(a_2\) is purely imaginary and both matrix products reduce to the identity matrix. The vanishing of \(a_{2,R}\) imposes a constraint on the value of \(\beta\) with \(-\beta(S_2 - S_3) = (n + 1/2)\pi\), and thus \(\alpha = 1/\beta = (n + 1/2)\pi/(S_2 - S_3) \approx (n + 1/2)1.47\). This condition is independent of the choice of the arbitrary constant term in \(S^2(z)\) since it depends only on the difference of \(S\) at two different points. We compare this quantization condition with numerically determined magic angles in Fig. 3(a).

The relative error \(\delta = (\alpha^{\text{WKB}}_n - \alpha^{\text{Num}}_n)/\alpha^{\text{Num}}_n\) is shown in the inset and becomes very small in small twist-angle limit. The magic-angle difference \(\alpha_{n+1} - \alpha_n\) is plotted in Fig. 3(b) and approaches the WKB result very closely at large \(n\).

At a given \(\beta\), the wavefunction of zero-energy state can be obtained by gluing the local solutions together via the connection formula. Specifically, by considering only \(e^{iS/\beta}\) component in region I, we find that the coefficients \(C_{A,B}\) at point 3 and point 1 are equal up to a phase factor \(e^{iA_0(x_3 - x_1)/\beta}\) with \(x_i\) being the \(x\)-coordinate of point \(i\). This indicates that the wavefunctions in the regions around points 1 and 3 are identical apart from the universal phase factor. Similarly, we find that the wavefunction around point 5 is the same as that around point 1 without phase difference since the connection figure.
matrix $T_{60} T_{61}$ is an identity matrix. By repeating this procedure, one can obtain a wavefunction over the two-dimensional plane, which is invariant under translation by a moiré lattice vector up to a phase. Such a phase contributes to a Bloch wavevector $(A_0/\beta, 0)$. A similar Bloch state can be obtained by considering only $e^{-ik y}$ in region 1 with the coefficients contributing a wavevector $(-A_0/\beta, 0)$. Both total wavevectors show vanishing components along $y$ and are therefore distinct from the zero-energy states at the moiré Brillouin-zone corners $K/K'$, which occur at all twist angles and have nonzero $k_y$.

We have identified additional values of $\beta$ at which the matrix products have unit eigenvalues and are tridiagonal with a nonzero off-diagonal matrix element. In this case, only $C_A$ can be nonzero at both AB and BA stacking points, in conflict with the $T_{12}$ connection formula $T_{12}$ which requires a $C_B$ at point 1 if nonzero $C_A$ appears at point 2. Therefore, these solutions are discarded.

**Summary and discussion.** In summary, we have studied the chiral symmetric model of twisted bilayer graphene, which can be viewed as describing a Dirac fermion in a non-dynamic nonabelian gauge field. By parameterizing the twist angle as a dimensionless effective Planck constant $\beta$, we provide a WKB solution to the zero-energy wave equation valid in the semiclassical limit where the gauge potential is non-zero. The zero-gauge-potential turning points, where the WKB approximation ceases to be valid, are located at the high symmetry moiré pattern points with local AB/BA/AA stacking. We obtain a global wavefunction by linearizing the gauge potential at the AB and BA points, expanding the local wavefunction in terms of Airy functions, and matching Airy functions with WKB solutions in their overlapping validity regions. For a general $\beta$, these global wavefunctions are multi-valued, exhibiting a topological obstruction. The single-valued property of a well-defined wavefunction leads to a constraint on the effective Planck constant $\beta = 1/\alpha$ so that physical zero-energy solutions are obtained at a discrete set of equally spaced $\alpha$. We find that these conditions are very close to the numerical values of $\alpha$ at which flat bands occur in numerical calculations.

By rotating the branch cuts by $\pm 2\pi/3$, additional zero-energy states appear, also at wavevectors away from the moiré band Dirac points which are known to have zero-energy eigenvalues at all twist angles. Because we have only found a finite number of zero-energy states, our work establishes only a necessary condition for the presence of zero-energy flat bands. The semi-classical interpretation of the sufficient condition for flat bands deserves further investigation.

We comment that the limited number of zero-energy solutions might be rooted in the assumption of a non-singular $S$. By relaxing the boundedness condition on $S$ used to fix the free analytical function $S^c(z)$, an additional periodic part can be added besides the $A_0 z$ part. The resulting wavefunction can still be well-defined if the unique wavefunction obtained above has zero amplitudes at the singular points and cancel the $S^c(z)$ singularity, following the idea from Tarnopolsky et al. However, our WKB solutions have difficulty in locating zero-points since they are approximate solution valid only to leading order in $\beta$. Nevertheless, our analysis can be regarded as an alternative support to the inevitability of the singularity in the wavefunctions of zero-energy flat bands.

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In this part, we describe the derivation of the Hamiltonian $H = (p + \alpha A) \cdot \sigma$ and show the wavevector of our approximate WKB wavefunction. We also present the asymptotic expansion coefficients here as shown in Fig. [6].

In the absence of intra-sublattice hopping, the Hamiltonian exhibits chiral symmetry. Under the basis functions of $\{|a, A\}, \{|t, A\}, \{|b, B\}, \{|t, B\}\}$ where $b/t$ indicate the top or bottom layer and $A/B$ is the sublattice index, the Hamiltonian reads

$$\mathcal{H}_0 = \begin{bmatrix} 0 & D_0^\dagger(r) \\ D_0(r) & 0 \end{bmatrix},$$

and

$$D_0(r) = \hbar v_F k_\theta \begin{bmatrix} (-2i\tilde{\partial} - \kappa_0)/k_\theta & \alpha U_0(r) \\ \alpha U_0(-r) & (-2i\tilde{\partial} - \kappa_1)/k_\theta \end{bmatrix}$$

where $v_F$ is the Fermi velocity of graphene, $k_\theta = 2k_D \sin(\theta/2)$ with $k_D = 4\pi/(3a_0)$ being the distance of Dirac point from the center of graphene’s Brillouin zone and $a_0$ being lattice constant of graphene, $\tilde{\partial} = (\partial_x + i\partial_y)/2$ represents the partial differential of parameter $\tilde{\varepsilon} = x - iy$, $\kappa_i = \kappa_{l,x} + ik_{l,y}$ with the layer index being $l = t/b$ and $\kappa_i = (\kappa_{l,x}, \kappa_{l,y})$ being the corresponding corners of the moiré Brillouin zone $[1, 7]$. $\alpha = t_\perp/\hbar v_F k_\theta$ is the inter-layer hopping strength and the interlayer hopping between different sublattices reads

$$U_0(r) = 1 + e^{i\phi} e^{-i(q_2 - q_1)\cdot r} + e^{-i\phi} e^{-i(q_3 - q_1)\cdot r}$$

where $\phi = 2\pi/3$, moiré modulation vector $q_i = k_\theta(\cos(-7\pi/6 + i\phi), \sin(-7\pi/6 + i\phi))$ with $i = 1-3$. In the following, we take the units of length, wavevector, and energy as $1/k_\theta$, $\hbar k_\theta$, and $\hbar v_F k_\theta$, respectively, the Hamiltonian can be simplified with only one parameter $\alpha$ $[2]$.

To further simplify, the constant terms in the diagonal matrix elements can be removed by performing the gauge transformation that changes the reference of the momentum of bottom and top layers $[2]$

$$\mathcal{D}_1 = \mathcal{U}^\dagger \mathcal{D}_0 \mathcal{U} = \begin{bmatrix} -2i\tilde{\partial} & \alpha U(r) \\ \alpha U(-r) & -2i\tilde{\partial} \end{bmatrix}$$

where

$$\mathcal{U} = \begin{bmatrix} e^{i\kappa_1 r} & \\ e^{i\kappa_2 r} \end{bmatrix};$$

SUPPLEMENTAL MATERIAL

In the Supplementary Materials, we show the asymptotic expansion coefficients of Airy functions, derive the Hamiltonian employed in this work, and describe the origin of the additional wavevector $k_\phi$.
FIG. 6. Asymptotic expansion coefficients in different regions. These coefficients are for variable $\bar{z}$ with the argument of it’s conjugate $\text{arg} \ z \in [0, 2\pi)$. Dotted lines are Stokes lines.

and $U(r) = e^{i(\kappa_1 - \kappa_2)r}U_0(r) = e^{-iq_1 r}U_0(0)$. By solving the simplified single-parameter Hamiltonian, one can obtain a wavefunction which, however, is not a Bloch wavefunction of the moiré lattice as the translation symmetry of $D_1$ is different from the moiré lattice and one need to perform the inverse gauge transform shown in Eq. (13), which will leads to a plane wave part with wavevector $k_\nu = q_3 + q_1/2$. 