Zero flat band electronic modes of twisted bilayer graphene: 3/2 quantization magic-angle rule and the hidden connection with coherent Landau level states

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Flat band electronic modes in twisted graphene bilayers are responsible for superconducting and other highly correlated electron-electron phases. Although some hints were known of a possible connection between the lowest Landau level and zero flat band modes, it was not clear how such connection appears. Here the electronic behavior in twisted bilayer graphene is studied using the chiral model Hamiltonian. As a result it is proved that for high-order magic angles, the zero flat band modes converge into coherent Landau states with a dispersion $\sigma^2 = 1/3\alpha$, where $\alpha$ is a coupling parameter that incorporates the twist angle and energetic scales. Then it is proved that the square of the Hamiltonian, which is a $2 \times 2$ matrix operator, turns out to be equivalent to a two-dimensional quantum harmonic oscillator. The interlayer currents between graphene’s bipartite lattices are identified with the angular momentum term while the confinement potential is an effective quadratic potential. From there it is proved a limiting quantization rule for high-order magic angles, i.e., $\sigma_{m+1} - \sigma_m = (3/2)m$ where $m$ is the order of the angle. All these results are in very good agreement with numerical calculations.

In 2018 it was found experimentally that twisted bilayer graphene (TBG) presents strongly correlated electron-electron quantum phases leading for example to unconventional superconductivity and Mott insulator states [1]. More recently, trilayer twisted graphene has been found to be the most strongly interacting correlated material [2, 3]. Such remarkable discoveries presented a new paradigm in the so-called Moiré materials and unveiled the importance of two-dimensional (2D) materials to understand unconventional superconductivity in cuprates and heavy fermions systems, as they share similar quantum phase diagrams [1, 2, 4]. TBG advantages are i) its simplicity, as they are made from a single chemical element, and ii) they have a high degree of manipulation that cuprates doesn’t have. In recent years, there has been a significant interest in these phases of matter from a fundamental point of view [5–13] but also because they present a lot of possible electronic applications and quantum computing advantages [13, 14]. There is also an interest connection between topological phases, edge states, semimetals and fractional quantum Hall effect (FQHE) [15–25]. A recently paper establishes a connection between heavy fermion models and TBG [4], opening the prospect of using heavy fermions physics to the superconducting physics of TBG and more strongly correlated phases.

The discovery of such phases was proceeded by the Bistritzer-Mac Donald (BM) theoretical observation that twisted bilayer graphene (TBG) develops flat bands at certain twisting angles which are called magic [26]. BM considered a continuum Dirac model in which the Moiré periodicity between layers produce Moiré Bloch bands [26]. The model is continuum in the sense that the interlayer potential between Carbon $\pi$ orbitals is a smooth function of the spacial separation projected onto the graphene planes and also the hopping is local and periodic, allowing to apply the Bloch’s theorem for any rotation angle. For TBG it was demonstrated that non-Abelian gauge fields arise due to the coupling between layers in the low-energy regime [27, 28].

Flat band modes which arise at magic angle, also known as zero energy modes, have been investigated in many recent works [29–38], and in particular, there were hints in the mathematics for a possible connection with the quantum Hall effect (QHE) and the lowest Landau level [29, 32]. There are interesting properties of the zero mode wave function [32–34], in particular, the connection with the lowest Landau level reveals that TBG presents topological phases [32, 39].

Importantly, the wave function is reminiscent of a quantum hall wave function because is described in terms of Jacobi theta functions such as in the quantum hall effect wave function [29–31]. This hidden wave function is important to understand because leads to particular localization properties, orbital current, density wave function distribution and symmetries of the pseudo-magnetic gauge fields. Yet, exactly how this analogy arises was not clear, as no connection between the quantum harmonic oscillator and the TBG hamiltonian was ever found. Tarnopolsky et. al. also found that magic angles were quantized but no explanation was provided for this fact [29]. Here we solve both problems and moreover, we find that in fact the zero flat band modes converge into coherent Landau levels. As we will discuss, this is done by using boundary layer differential equations theory and squaring the Hamiltonian [28, 40–43].

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The chiral Hamiltonian of twisted bilayer graphene is a variant of the original Bistritzer-MacDonald Hamiltonian in which the $AA$ tunneling is set to zero [31]. Here we use as basis the wave vectors $\Phi(r) = (\psi_1(r), \psi_2(r), \chi_1(r), \chi_2(r))^T$ where the index 1, 2 represents each graphene layer and $\psi_1(r)$ and $\chi_2(r)$ are the Wannier orbitals on each inequivalent site of the graphene's unit cell. The chiral Hamiltonian is given as

$$H = \left( \begin{array}{cc} 0 & D(r) \\ D^*(r) & 0 \end{array} \right)$$

(1)

where the zero-mode operator is defined as,

$$D(r) = \left( \begin{array}{cc} -i\tilde{\alpha} & aU(r) \\ aU(-r) & i\tilde{\alpha} \end{array} \right)$$

(2)

and,

$$D^*(-r) = \left( \begin{array}{cc} -i\tilde{\alpha} & aU^*(-r) \\ aU^*(r) & i\tilde{\alpha} \end{array} \right)$$

(3)

with $\tilde{\alpha} = \tilde{\alpha}_x + i\tilde{\alpha}_y$, $\tilde{\alpha} = \tilde{\alpha}_x - i\tilde{\alpha}_y$. The potential is,

$$U(r) = e^{-i\phi_1} + e^{i\phi_2} + e^{i\phi_3}$$

(4)

where the phase factor $\phi = 2\pi/3$ and the Moiré lattice vectors are given by $q_1 = k_0(0, 1)$, $q_2 = k_0(\sqrt{3}, 0)$, $q_3 = k_0(\sqrt{3}, 2\sqrt{3})$, where the Moiré modulation vector is $k_0 = 2k_D \sin \frac{\theta}{2}$ with $k_D = 2\sqrt{3}$ is the magnitude of the Dirac wave vector and $\theta = 30\degree$ is the lattice constant of monolayer graphene. The model contains only the parameter $\alpha$, defined as $\alpha = \frac{w_3}{w_1k_0}$ where $w_3$ is the interlayer coupling of stacking AB/BA with value $w_1 = 110$ meV and $v_0$ is the Fermi velocity with value $v_0 = 1.9816\times W_1$. The operators $\tilde{\alpha}$ and $\tilde{\alpha}$ are dimensionless as the Hamiltonian Eq. (1) is written in using units where $\tilde{\alpha}_x = 1$, $\tilde{\alpha}_y = 1$. The twist angle only enters in the dimensionless parameter $\alpha$. The combinations $b_{1,2} = q_{1,2} - q_1$ are the Moiré Brillouin zone (mBZ) vectors and also $b_3 = q_3 - q_2$. Using this basis for the reciprocal space lattice, some important high symmetry points of the Moiré Brillouin zone are $K = (0, 0)$, $K' = -q_1$, and $\Gamma = q_1$ (see ref. [40] for a diagram). For further use it is also convenient to define a set of unitary vectors $\hat{q}_{1}^\perp$ perpendicular to the set $q_{m}$ and given by $\hat{q}_{1}^\perp = (1, 0)$, $\hat{q}_{2}^\perp = (-1/2, \sqrt{3}/2)$, $\hat{q}_{3}^\perp = (-1/2, -\sqrt{3}/2)$.

In a previous work we showed how, by taking the square of $H$, it is possible to write the Hamiltonian as a $2 \times 2$ matrix [28, 40],

$$H^2 = \left( \begin{array}{cc} -\nabla^2 + \alpha^2(U(r))^2 & \alpha A^1(r) \\ \alpha A^1(r) & -\nabla^2 + \alpha^2(U(r))^2 \end{array} \right)$$

(5)

where the squared norm of the potential is an effective trigonal confinement potential,

$$|U(r)|^2 = 3 + 2\cos(b_1 \cdot r - \phi) + 2\cos(b_2 \cdot r + \phi)$$

$$+ 2\cos(b_3 \cdot r + 2\phi)$$

(6)

and the off-diagonal term is,

$$A^1(r) = -i \sum_{\mu=1}^{3} e^{-i\hat{q}_{\mu} \cdot r} (2\hat{q}_{\mu} \cdot \nabla + 1)$$

(7)

where $\nabla^\perp = -\nabla$ with $\nabla = (\partial_x, \partial_y)$ and $\mu = 1, 2, 3$.

Now we investigate the asymptotic limit $\alpha \to \infty$ by numerically solving (see supplementary) the Schrödinger equation $H \psi(r) = E \psi(r)$ where $E$ is the energy. As the potential is periodic, it satisfies Bøch’s theorem and thus $\psi_{k,j}(r) = e^{i\beta r} u_{k,j}(r)$ where $u_{k,j}(r)$ has the periodicity of the lattice (see supplementary). In Fig. 1 we present the zero mode wave function, corresponding to $E = 0$ at the reciprocal space point $k = \Gamma$ for the m-esim magic angles ($\alpha_m$) with $m = 8$ and $m = 9$. The electronic maxima of the density form hexagons which are nearly localized at $r_\mu \approx q_\mu$. Such observation is detailed in Fig. 1. Moreover, the wave-function for other $k$ points follow the same behavior although the $\Gamma$ point best captures the magic angle behavior [40]. In the limit of $\alpha_m \to \infty$ we have verified that in fact, the electron density is almost localized at $q_\mu$. Notice that here we are working with adimensional units but this suggests a connection with the QHE as solutions seem self-dual [45], i.e., in real space are similar to those in reciprocal space with renormalized parameters.

Although there are expressions for the wave-function [29, 33, 46] at any $k$ point that hinted a relationship with the lowest Landau levels, they depend on the wave function at the $K$ point, i.e.,

$$\psi_{k,j}(r) = f_k(z) \psi_{K,j}(r)$$

(8)

where $z = x + iy$ and $f_k(z)$ is an analytic function which satisfy the boundary condition and turns out to be a Jacobi theta function. The form of the $\psi_{K,j}(r)$ is not analytically known. Yet in Figs. 1 and 2 we see numerically that the electron wave function reaches an asymptotic limit almost invariant as $\alpha_m \to \infty$ and does not depend much on $k$. This wave function tends to be localized in certain points of space which are not the stacking points AA, AB and BA. In that sense, the solutions are different from the first magic angle a fact that was explained elsewhere [40].

To understand how this limiting wave function arises, let us discuss the zero-mode equation

$$D(r) (\psi_1(r), \psi_2(r))^T = 0.$$  

Although not essential for the analysis, it is easier to understand the $\Gamma$ point solution. For this case we have that due to symmetry, $\psi_2(r) = i\mu_\alpha \psi_1(-r)$ where $\mu_\alpha = \pm 1$ depending on the magic angle parity [29]. Therefore, we obtain,

$$\tilde{\partial} \psi_1(r) = \alpha \mu_\alpha U(r) \psi_1(-r)$$

(9)

$$\tilde{\partial} \psi_1(-r) = -\alpha \mu_\alpha U(-r) \psi_1(r)$$

(10)

To solve the equation in the limit $\alpha \to \infty$ we use the boundary layer theory of differential equations [47], i.e.,
FIG. 1. Wave function localization for some high-order magic angles at \( k = \Gamma \). In Panels a) and b) we present the real (orange curves) and imaginary (purple curves) parts of the wave function at the symmetric line \((0, y)\) for layer 1 and layer 2 at magic angles \( \alpha_8 = 11.345 \) and \( \alpha_9 = 12.855 \) respectively. Panels c) and d), contour plot of the global electronic density \( \rho_1(r) + \rho_2(r) \) for \( \alpha_8 = 11.345 \) and \( \alpha_9 = 12.855 \) respectively. The vertical line (yellow line) inside the Wigner-Seitz cell indicates the cut along the \( y \) axis used in panel a) and b). The external hexagon is the Wigner-Seitz cell, where the AB (green), BA (yellow) and AA (red) stacking points are indicated. For higher magic angles, the wave-function density localizes in 6 high density points, located at \( r = \pm q_\mu \), with \( \mu = 1, 2, 3 \), forming the red spots of maximal density.

whenever the gradients are small, we can neglect the derivative in Eqns. (9)-(10) when compared to the potential term. Then our solution must satisfy \( \psi_j(r) \to 0 \). The solution will be different from zero only inside the boundary layer, i.e., whenever \( \partial \psi_j(r) \) is of order \( aU(\pm r)\psi_j(r) \). Taken into account the boundary layer we conclude that the solution must be strongly peaked around certain regions of space. Then is natural to seek the solution within continuous functions having a peak while keeping the form of Eq. (8). We then propose a coherent Landau state ansatz for a given layer (and thus supress the subindex \( j \)),

\[
\psi(z, z*) = f_\lambda(z)e^{-\frac{|z|^2}{2\sigma^2}} \tag{11}
\]

where \( f_\lambda(z) \) is an analytic function [48],

\[
f_\lambda(z) = \frac{1}{\sigma \sqrt{2\pi}} e^{\frac{z^2}{2\sigma^2}} \tag{12}
\]

The parameter \( \lambda \) is the localization center (known as the guiding coordinates in the QHE problem [49]) and \( \sigma \) the standard deviation as the electronic density is a Gaussian,

\[
\rho(r) = \frac{1}{2\pi \sigma^2} e^{-\frac{|z|^2}{2\sigma^2}} \tag{13}
\]

Notice how the Gaussian envelope in Eq. (11) ensures the boundary layer condition, i.e., the vanishing of the wave function whenever the gradient is small.

However, still we need to make remarks. As the equation involves \( \psi(r) \) and \( \psi(-r) \), the solutions can be written as a sum of a symmetrized and antisymmetrized forms. Therefore, it will be a linear combination of the symmetrized/antisymmetrized wavefunctions,

\[
\psi_\pm(z, z*) = e^{-\frac{|z|^2}{2\sigma^2}} \frac{1}{\sqrt{2}} (f_\lambda(z) \pm f_{-\lambda}(z)) \tag{14}
\]

provided that \( \lambda \) is far away from \(-\lambda\) to avoid overlap between the Gaussians centered at \( \lambda \) and \(-\lambda\). In what follows we will use our ansatz in the zero mode equation to prove how it satisfies the equation and to obtain \( \sigma \).

Before doing so, observe that \( \psi(r) \) must transform according to the \( C_3 \) symmetry group and this can be ensured by defining \( \lambda_1 \) such that,

\[
\psi_\pm(z, z*) = \frac{1}{\sqrt{6}} \sum_{\mu=1}^{3} e^{-\frac{|z|^2}{2\sigma^2}} (f_{\lambda_\mu}(z) \pm f_{-\lambda_\mu}(z)) \tag{15}
\]

where \( \lambda_2 = e^{i\phi}\lambda_1 \) and \( \lambda_3 = e^{-i\phi}\lambda_1 \) and the normalization constant was modified to account for two layers and the three \( \lambda_\mu \). Concerning the boundary conditions, i.e., the Bloch theorem, we will discuss the subject after testing the solution for a unit cell.

As the numerical simulation indicates that the electronic density is localized on \( \pm q_\mu \), this suggests to propose \( \lambda_\mu = Q_\mu = q_\mu^x + iq_\mu^y \) where \( q_\mu^x \) and \( q_\mu^y \) are the components of vector \( q_\mu = (q_\mu^x, q_\mu^y) \). Finally, the parameter \( \sigma \) will be determined by imposing the ansatz to satisfy Eqns. (9)-(10).

Now we test our ansatz in the zero mode equation. Using complex numbers and that \( \partial = 2 \frac{\partial}{\partial z^*} \), the zero mode equation can be rewritten as,

\[
\frac{\partial}{\partial z^*} \psi_\pm(z, z^*) = \mu_\alpha \sigma_m U(z, z^*) \psi_\pm(-z, -z^*) \tag{16}
\]

where \( \sigma_m \) indicate a magic angle and \( U(z, z^*) \) is the complex form of the coupling layer potential \( U(r) \).

In the limit \( \alpha \to \infty \) we can expand \( U(z, z^*) \) locally around \( Q_\mu \) (see supplementary) where the boundary layer lies, therefore,

\[
U(z, z^*) \psi_\pm(-z, -z^*) \approx \frac{3z}{2} \psi_\pm(-z, -z^*). \tag{17}
\]

Next we use that the anti-holomorphic derivative of an analytic function is zero from where

\[
\frac{\partial \psi_\pm(z, z^*)}{\partial z^*} = 2 \frac{\partial \psi_\pm(z, z^*)}{\partial z} = -\frac{z}{2\sigma^2} \psi_\pm(z, z^*) \tag{18}
\]

Finally, we combine the left-side of the zero mode equation, Eq. (18), with the right-hand side and use Eq. (17) to obtain,

\[
-\frac{z}{\sigma^2} \psi_\mp(z, z^*) \approx \mu_\alpha \sigma_m z \psi_\mp(z, z^*) \tag{19}
\]
where we see that the equation imposes the need of a symmetric or antisymmetric solution depending on the magic angle parity, given by the sign of \( \mu_\alpha \). This can be numerically verified in Fig. 1 although is seen that for finite \( \alpha \), the solution still is not purely symmetric or antisymmetric. Moreover, from Eq. (19) we obtain the width of the coherent Landau state,
\[
\lim_{m \to \infty} \sigma = \frac{1}{\sqrt{3} \alpha_m} \quad (20)
\]
To test these two results, in Fig. 2 we compare the evolution of the electronic density as \( \alpha \to \infty \) for several magic angles, in this case for the axis \( x = 0 \). The dashed line is the asymptotic solution given by Eq. (15) which does not contain any free parameter.

In Fig. 3 we show a log-log plot of \( \sigma \) versus \( \alpha_m \) as obtained by fitting Gaussians to the numerical results. The red line is the theoretical prediction given by Eq. (20) giving a very good agreement with the numerical data for higher order magic angles. In Fig. 3 b) we also plot the maximum position of the numerically obtained wavefunctions \( |r_m| \), confirming the tendency for localization seen in the inverse participation ratio \([40]\). This is why the ansatz almost obey the Bloch theorem, i.e., zero modes are akin to other confined states in which the overlap between wave functions at different unitary cells is almost zero \([28]\). In fact, the set of coherent Landau levels is overcomplete \([50]\).

By using complex notation for \( H^2 \), the symmetry relation between layer components wave function at the \( \Gamma \) point and Eq. (19) it follows that,
\[
\left( 4p_z p_z^* + \frac{3 \alpha}{2} |z|^2 - 3 \alpha L_z \right) \psi(z, z^*) = 0 \quad (22)
\]
where \( L_z = i(z p_z - z^* p_z^*) \) is the angular momentum and \( p_z = p_x - i p_y \) with \( p_j = -i \hbar \partial_j \) is the momentum operator. Moreover, we can define the creation/annihilation operator associated,
\[
a_z = \sqrt{\frac{3 \alpha}{4 \hbar}} z + \frac{2}{\sqrt{3 \alpha \hbar}} p_z^* \quad (23)
\]
\[
a_z^\dagger = \sqrt{\frac{3 \alpha}{4 \hbar}} z^* - \frac{2}{\sqrt{3 \alpha \hbar}} p_z \quad (24)
\]
from where we obtain an effective two-dimensional quantum harmonic oscillator Hamiltonian,
\[
H_{zz^*} \psi(z, z^*) = \left( \hbar \omega a_z^\dagger a_z + \omega L_z \right) \psi(z, z^*) \quad (25)
\]
with $\omega = 3\alpha$. Defining the conjugate operators $a_{z^*}$ and $a^\dagger_{z^*}$ (see suplementary), it follows that the angular momentum is,
\[ L_z = \frac{\hbar}{2}(a^\dagger_{z^*}a_z - a_{z^*}^\dagger a^\dagger_z) \] (26)
where $L^\dagger_z = L_z$ and therefore Eq. (25) is rewritten as,
\[ H_{zz^*}\psi(z, z^*) = \hbar\omega (N_{zz^*} + 1) \psi(z, z^*) \] (27)
where $N_{zz^*} = \frac{1}{2}(a_{z^*}^\dagger a_z^\dagger + a^\dagger_{z^*} a^\dagger_z)$ in analogy to a 2D harmonic oscillator. The constant term $\hbar\omega$ is the zero-point energy of the oscillator. Now is clear the $3/2$ quantization rule: they are just different oscillator levels as, although in Eq. (27) the levels are spaced by $\alpha = 3m$, we must remember that we have two equations, one for $m$ odd and $m$ even. Therefore, the $3m$ is the recurrence for each parity sequence and thus magic angles, without distinction of parity, occurs for $\alpha = (3/2)m$. Finally, we can compare Eq. (26) and the interlayer currents between bipartite layers that were investigated in a previous work [40]. Apart from a dimensional constant, both expressions coincide from where we can identify the angular moment with such currents. As explained elsewhere [40], magic angles have a precise kinetic, confinement energies and current balance.

In conclusion, we showed that the twisted bilayer hamiltonian can be reduced to a quantum harmonic oscillator and thus magic angles are quantized. Zero flat band modes converge into coherent Landau levels. Due to the multiple mathematical and physical properties of coherent states, this opens many exciting technological and physical possibilities in Moiré materials, as for example, the possibility of controlling coherency by manipulation of the twisting angle or the self-duality property of the wave functions [45].

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I. SUPPLEMENTARY MATERIAL

A. Wave-functions Fourier coefficients in reciprocal space

Here we use as basis the wave vectors $\Phi(r) = (\psi_1(r), \psi_2(r), \chi_1(r), \chi_2(r))^T$ where the index 1,2 represents each graphene layer and $\psi_j(r)$ and $\chi_j(r)$ are the Wannier orbitals on each inequivalent site of the graphene’s unit cell.

A general Bloch’s wave function with momentum $k$ in the mBZ at each sublattice has the form

$$\Psi_k(r) = \begin{pmatrix} \psi_{k,1}(r) \\ \psi_{k,2}(r) \end{pmatrix} = \sum_{mn} \left( \begin{array}{c} a_{mn} \\ b_{mn} \end{array} \right) e^{i(K_{mn}+k) \cdot r}$$

$$\chi_k(r) = \begin{pmatrix} \chi_{k,1}(r) \\ \chi_{k,2}(r) \end{pmatrix} = \sum_{mn} \left( \begin{array}{c} c_{mn} \\ d_{mn} \end{array} \right) e^{i(K_{mn}+k) \cdot r}$$

where $a_{mn}$ and $b_{mn}$ are the Fourier coefficients of layer 1 (layer 2) for sublattice A and $c_{mn}$ and $d_{mn}$ are the Fourier coefficients of layer 1 (layer 2) for sublattice B, and $K_{mn} = mb_1 + nb_2$ with $b_{1,2}$ are the two Moiré Brillouin zone vectors. If we substitute Eq. (1) and Eq. (2) into $\mathcal{H}\Psi_k(r) = E\Psi_k(r)$ we can calculate the eigenfunctions of $\mathcal{H}$,

$$K_{mn}^x a_{mn} + \alpha(b_{mn} + e^{i\phi} b_{m+1,n} + e^{-i\phi} b_{m,n+1}) = E a_{mn}$$

(3)

$$K_{mn}^x a_{mn} + \alpha(b_{mn} + e^{i\phi} b_{m-1,n} + e^{-i\phi} b_{m,n-1}) = E b_{mn}$$

(4)

$$K_{mn}^y c_{mn} + \alpha(d_{mn} + e^{-i\phi} d_{m+1,n} + e^{i\phi} d_{m,n+1}) = E c_{mn}$$

(5)

$$K_{mn}^y c_{mn} + \alpha(d_{mn} + e^{-i\phi} d_{m-1,n} + e^{i\phi} d_{m,n-1}) = E d_{mn}$$

(6)

where $K_{mn} = K_{mn} + k$.

Here Eqs. (3-6) form a coupled linear system that can be solved to find the corresponding eigenvalues. In general, there are $L = (2N + 1) \times (2N + 1)$ coefficients with $N$ the range of the matrix and $2N + 1$ the elements in the set, therefore, the Hamiltonian matrix has dimension $D = 4L$. In a similar way we can obtain the eigenfunctions of $H^2$ but the system is easier write as the matrix is only of size $2 \times 2$. Observe that all eigenfunctions of $\mathcal{H}$ are always eigenfunctions of $H^2$ but the converse is not true. This was discussed in detail elsewhere [1].

The system can be further reduced by using the $C_3$ symmetry. We denote the corresponding rotational operators $R_\phi$ and $R_{2\phi}$ by the angle $\phi$ and $2\phi$ respectively. Their matrix representations $D_\phi$. $D_{2\phi}$ and the identity, have eigenvalues $w = \{ 1, e^{i\phi}, e^{-i\phi} \}$. Eigenfunctions of the Hamiltonian are also eigenfunctions of such operators, and thus we have the relation $\psi_k(R_{2\phi}(r)) = e^{i\phi}\psi_k(r)$ and $\psi_k(R_\phi(r)) = e^{-i\phi}\psi_k(r)$, with the property $R_\phi(q_{\mu}) \cdot r = q_{\mu} \cdot R_\phi^{-1}(r)$. One can obtain a relationship between coefficients using such rotations to reduce the problem into a one trigonal sector.

To perform such calculation, it is very useful to have the Moiré reciprocal basis vector transformation rules under the rotations. We reproduce below such useful rules,

$$R_\phi(b_1) = b_2 - b_1$$

$$R_\phi(b_2) = -b_1$$

$$R_{2\phi}(b_1) = -b_2 + b_1$$

(7)

FIG. 1. Moiré vectors rotational $C_3$ rules. The operator $R_\phi$ rotate by $\phi = \frac{2\pi}{3}$ moiré vectors $b_1$ ($b_2$) indicated by purple (green) arrows.

B. Fourier coefficients in Γ-point reciprocal

In the $\Gamma$ point, using the symmetry of the Hamiltonian it can be proved that the spinor components are related through $\psi_\Gamma(r) = i\mu_\psi \psi_{\Gamma,\Gamma}(-r)$. Tarnoposky et. al [2] found that,

$$\partial \psi_{\Gamma,1}(r) = \alpha U(r) \psi_{\Gamma,1}(-r) = E_{\Gamma} \psi_{\Gamma,1}(-x, y)$$

(8)

Following this analysis a reduced equation for the Fourier coefficients can be written as,

$$[K_{mn} + q_1] e^{i\phi(K_{mn} + q_1)a_{mn}} = \alpha(a_{mn} + e^{i\phi}a_{m,-n+1} + e^{-i\phi}a_{m+1,n-1}) = E_{\Gamma} a_{mn}$$

(9)
From the $\Gamma = q_1$ point the symmetry of the component of the spinors $\psi_2, r(r) = i\mu_\alpha \psi_1, r(-r)$, we found the following relation,

$$\sum_{m,n} b_{mn} e^{i(K_{mn} + 2q_1) \cdot r} = i\mu_\alpha \sum_{m',n'} a_{m'n'} e^{-i(K_{m'n'} + q_1) \cdot r}$$

or simplifying,

$$\sum_{m,n} b_{mn} e^{iK_{mn} \cdot r} = i\mu_\alpha \sum_{m',n'} a_{m'n'} e^{-i(K_{m'n'} - 3q_1) \cdot r}$$

note that $b_1 + b_2 = -3q_1$ and Eq. (11) is rewritten as,

$$\sum_{m,n} b_{mn} e^{iK_{mn} \cdot r} = i\mu_\alpha \sum_{m',n'} a_{m'n'} e^{iK_{m',1-n'} \cdot r}$$

change index $m = 1 - m' \rightarrow m' = 1 - m$ and $n = 1 - n' \rightarrow n' = 1 - n$ in Eq. (12), therefore,

$$\sum_{m,n} (b_{mn} - i\mu_\alpha a_{1-m,1-n}) e^{iK_{mn} \cdot r} = 0$$

Finally, the relation between Fourier coefficients of each layer in the $\Gamma$ point is simply,

$$b_{mn} = i\mu_\alpha a_{1-m,1-n}$$

with $\mu_\alpha = \pm 1$ and also follows that,

$$\text{Re}\{b_{mn}\} = -\mu_\alpha \text{Im}\{a_{1-m,1-n}\}$$

and

$$\text{Im}\{b_{mn}\} = \mu_\alpha \text{Re}\{a_{1-m,1-n}\}$$

Using the $C_3$ symmetry of the wave-function at the $\Gamma$-point, $k = q_1$,

$$\Psi(R_\phi(r)) = \sum_{m,n} \left( b_{mn} e^{iR_\phi(m b_1 + n b_2 + q_1) \cdot r} \right) e^{iR_\phi(m b_1 + n b_2 + q_1) \cdot r}$$

where $mR_\phi(b_1) + nR_\phi(b_2) + R_\phi(q_1) = m(b_2 - b_1) + n(-b_2) + q_2$. From the rotated vectors in Eq. (17) follows that,

$$\sum_{m,n} a_{mn} e^{i(m b_1 + n b_2) \cdot r} = e^{i\phi} \sum_{m,n} a_{mn} e^{i(-m-n+1)b_1 + m b_2) \cdot r}$$

using new index $m' = -m - n + 1 \rightarrow n = 1 - m' - n'$ and $n' = m$ follows that,

$$\sum_{m,n} a_{mn} e^{i(m b_1 + n b_2) \cdot r} = e^{i\phi} \sum_{m,n} a_{m',1-m'-n'} e^{i(m' b_1 + n' b_2) \cdot r}$$

therefore,

$$e^{-i\phi} a_{mn} = a_{n,-m-n+1}$$

and,

$$e^{i\phi} a_{mn} = a_{-m-n+1,m}$$

using this last $C_3$ symmetry in (8) at the magic angles follows that,

$$\left( \frac{i\sqrt{3}}{2}(m-n) + \frac{3}{2}(m+n) \right) a_{m,n} \mp \alpha_m (a_{1-m,1-n} + a_{-m-n+n + a_{m+n,-m}} = 0$$

where $K_{mn} = m b_1 + n b_2 = (\sqrt{\frac{3}{2}}(m-n), \frac{3}{2}(m+n) - 1)$ is the Moiré reciprocal vector.

C. Coherent Landau level solution in the limit $\alpha \rightarrow \infty$

Consider a coherent state of the form,

$$\psi(z, z^*) = f_\lambda(z) e^{-\frac{i\pi}{4\sigma^2}|z|^2}$$

$$= \frac{1}{\sigma \sqrt{2\pi}} e^{i\lambda^* z} e^{-\frac{1}{4\sigma^2}|\lambda^*|^2 \cdot \frac{i\lambda^*}{4\sigma^2}|z|^2}$$

The complete form of wave function is obtained by summing over the contributions for $\lambda$ and $-\lambda$,

$$\psi_{\pm}(z, z^*) = \frac{1}{\sqrt{2}} \left( f_\lambda(z) e^{-\frac{i\pi}{4\sigma^2}|z|^2 \mp f_{-\lambda}(z) e^{-\frac{i\pi}{4\sigma^2}|z|^2} \right)$$

$$= \frac{1}{\sigma \sqrt{2\pi}} \left( e^{i\frac{1}{4\sigma^2} \lambda^* z - \frac{1}{4\sigma^2} \lambda^* z - \frac{1}{4\sigma^2} |z|^2} = e^{-\frac{i\pi}{4\sigma^2} \lambda^* z - \frac{1}{4\sigma^2} \lambda^* z - \frac{1}{4\sigma^2} |z|^2} \right)$$

where $\lambda$ is the center of the Gaussians. Is important to note that Eq. (24), satisfies the relation $\psi_{\mp}(-z, -z^*) = \pm \psi_{\pm}(z, z^*)$ as we consider here the wavefunction as a sum of symmetrized/antisymmetrized functions that can be treated separately. We also have,

$$|\psi_{\pm}(z, z^*)|^2 \approx \frac{1}{2\sigma^2 (2\pi)} \left( e^{-\frac{i\pi}{4\sigma^2} |z-\lambda|^2} + e^{-\frac{i\pi}{4\sigma^2} |z+\lambda|^2} \right)$$

where the overlap term between Gaussian’s is neglected in the limit $\alpha \rightarrow \infty$. On the other hand, the coupling potential can be written as,

$$U(z, z^*) = -\frac{2}{\sqrt{\sigma^2}} S(z, z^*)$$

where $\tilde{\sigma} = 2\sqrt{\sigma^2}$ and,

$$S(z, z^*) = \sum_{\mu=1}^{3} e^{-i(Q_{\mu}^* z + Q_{\mu} z^*)/2}$$
where $Q_\mu = q_\mu^* + i q_\mu$. Therefore,

$$\frac{\partial}{\partial z^*} S(z, z^*) = \frac{1}{2} \sum_{\mu=1}^{3} (-iQ_\mu)e^{-i(Q_\mu^*z + Q_\mu z^*)/2}$$

(28)

Finally, $U(z, z^*)$ is the complex form of the coupling layer potential,

$$U(r) = U(z, z^*) = \sum_{\mu=1}^{3} (iQ_\mu)e^{-i(Q_\mu^*z + Q_\mu z^*)/2}$$

(29)

Notice that such result can be obtained straightforward from the definition of $U(r)$ and $z$ and $z^*$, yet is illustrative to use the function $S(z, z^*)$ as this quantity appears in several commutators [1].

Substituting Eqns. (26)-(28) in Eq. (8) for magic angles,

$$2 \frac{\partial}{\partial z^*} \psi_\pm(z, z^*) = \pm \alpha_m (-2 \frac{\partial}{\partial z} S(z, z^*)) \psi_\pm(-z, -z^*)$$

$$= \pm \alpha_m \left( \sum_{\mu=1}^{3} (iQ_\mu)e^{-i(Q_\mu^*z + Q_\mu z^*)/2} \right) \psi_\pm(-z, -z^*)$$

(30)

using the fact that in the limit $\alpha \rightarrow \infty$ the wave function is localized in $Q_\mu$, and in other points is zero, we can expand (30) around $Q_\mu$ up to first order,

$$2 \frac{\partial}{\partial z^*} \psi_\pm(z, z^*) \approx \pm \alpha_m \left( \sum_{\mu=1}^{3} (iQ_\mu)(1 - \frac{i}{2}Q_\mu z^* + Q_\mu z^*) \right) \psi_\pm(-z, -z^*)$$

(31)

and since $\sum_{\mu} Q_\mu = \sum_{\mu} Q_\mu^* = 0$ and $\sum_{\mu} |Q_\mu|^2 = 3$, it follows that,

$$2 \frac{\partial}{\partial z^*} \psi_\pm(z, z^*) \approx \left( \frac{3\alpha_m}{2} \right) \psi_\pm(-z, -z^*)$$

(32)

since $\psi_\pm(z, z^*) = \mp \psi_\mp(-z, -z^*)$. Normalizing, the final form of the ansatz wave function for $\alpha \rightarrow \infty$ is,

$$\psi_\pm(z, z^*) = \frac{1}{\sqrt{2\pi}} \sum_{\mu=1}^{3} (fQ_\mu(z)e^{-\frac{1}{2}x^2|z|^2}$$

(33)

$$\pm fQ_\mu(z)e^{-\frac{1}{2}x^2|z|^2})$$

From the square Hamiltonian at the zero flat band $H^2\Psi(r) = 0$ it follows that,

$$(-\nabla^2 + \alpha^2 |U(-r)|^2) \psi_1(r) + \alpha A^\dagger_1(r) \psi_2(r) = 0$$

rewritten in complex notation,

$$(4p_z^2 + \left( \frac{3\alpha}{2} \right)^2 |z|^2) \psi(z, z^*) + i\mu_\alpha \alpha A^\dagger_1(z, z^*) \psi(-z, -z^*) = 0$$

(35)

where $A^\dagger_1(r) \approx -2i \sum_{\mu=1}^{3} e^{-iQ_\mu^* \cdot \nabla} \Psi_{z^*}$ for $\alpha \rightarrow \infty$ [3], therefore,

$$A^\dagger_1(z, z^*) \psi(-z, -z^*) = -2i \sum_{\mu=1}^{3} e^{-\frac{i}{2}(Q_\mu^*z + Q_\mu z^*)}(Q_\mu^* \cdot \nabla)$$

$$+ Q_\mu^* \partial_z \psi(-z, -z^*)$$

(36)

now for $\alpha \rightarrow \infty$ we expand locally around $Q_\mu$ where the boundary layer lies and considering that $Q_\mu^* = iQ_\mu$, it follows that

$$A^\dagger_1(z, z^*) \psi(-z, -z^*) = -2i \sum_{\mu=1}^{3} (1 - \frac{i}{2}Q_\mu z^* + Q_\mu z^*)(iQ_\mu \partial_z$$

$$- iQ_\mu^* \partial_{z^*} \psi(-z, -z^*)$$

(37)

with $\sum_{\mu=1}^{3} Q_\mu = 0$ and $\sum_{\mu=1}^{3} |Q_\mu|^2 = 3$ we have that,

$$A^\dagger_1(z, z^*) \psi(-z, -z^*) = -3i(z\partial_z - z^*\partial_{z^*}) \psi(-z, -z^*)$$

$$= 3(zp_z - z^*p_{z^*}) \psi(-z, -z^*)$$

(38)

substituting Eq. (38) in Eq. (35),

$$(4p_z^2 + \left( \frac{3\alpha}{2} \right)^2 |z|^2) \psi(z, z^*) + 3\mu_\alpha \alpha(zp_z$$

$$- z^*p_{z^*}) \psi(-z, -z^*) = 0$$

(39)

however the angular momentum in complex notation is defined as $L_z = i(zp_z - z^*p_{z^*})$ and we have that,

$$(4p_z^2 + \left( \frac{3\alpha}{2} \right)^2 |z|^2) \psi(z, z^*) + 3\alpha L_z \mu_\alpha \psi(-z, -z^*) = 0$$

(40)

for odd parity $\mu_\alpha = 1$ the solution is anti-symmetric $\psi(-z, -z^*) = -\psi(z, z^*)$ and for even parity $\mu_\alpha = -1$ the solution is symmetric $\psi(-z, -z^*) = \psi(z, z^*)$. Therefore, the equation is reduced as,

$$(4p_z^2 + \left( \frac{3\alpha}{2} \right)^2 |z|^2 - 3\alpha L_z) \psi(z, z^*) = 0$$

(41)

On the other hand, the quantum harmonic oscillator in complex notation is,

$$H_{z,z^*} \psi(z, z^*) = \left( \frac{2p_z^2 + \left( \frac{3\alpha}{2} \right)^2 |z|^2}{m} \right) \psi(z, z^*)$$

(42)

from where we identified by comparison with 41 that $m = \frac{1}{2}$ and $\omega = 3\alpha$, therefore we can define a creation/annihilation operators associated as,

$$a_z = \sqrt{\frac{3\alpha}{4\hbar}} z + i \frac{2}{\sqrt{3\alpha\hbar}} p_z$$

(43)
\[
a^\dagger_z = \sqrt{\frac{3\alpha}{4\hbar}} - i \frac{2}{\sqrt{3\alpha} \hbar} p_z \quad (44)
\]
from where,
\[
a^\dagger_z a_z = \frac{3\alpha}{4\hbar} |z|^2 + 4p_z p_z^* + i \frac{2}{\sqrt{3\alpha} \hbar} \sqrt{3\alpha} \hbar (z^* p_z^* - z p_z)
\]
multiplying both sides of Eq. (45) by 3 follows that
\[
\hbar (3\alpha) a^\dagger_z a_z = \left(\frac{3\alpha}{2\hbar}\right)^2 |z|^2 + 4p_z p_z^* - 3\alpha L_z
\]
from where we obtain an effective two-dimensional quantum harmonic oscillator Hamiltonian,
\[
H_{zz^*} \psi(z, z^*) = \left(\hbar \omega a^\dagger_z a_z + \omega L_z\right) \psi(z, z^*) \quad (47)
\]
where \(L_z = \frac{\hbar}{2}(a^\dagger_z a_{z^*} - a^\dagger_{z^*} a_z)\) is Hermitian and therefore Eq. (47) is rewritten as,
\[
H_{zz^*} \psi(z, z^*) = \hbar \omega (N_{zz^*} + 1) \psi(z, z^*) \quad (51)
\]
with \(N_{zz^*} = \frac{1}{2}(a^\dagger_z a_{z^*} + a^\dagger_{z^*} a_z) = \frac{1}{2}(N_z + N_{z^*})\) with \(N_z = a^\dagger_z a_z\) and \(N_{z^*} = a^\dagger_{z^*} a_z\) in analogy to a 2D harmonic oscillator where \(\omega = 3\alpha\). The constant term \(\hbar \omega\) is the zero-point energy of the oscillator.

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