Magic angles in twisted bilayer graphene near commensuration: towards a hyper-magic manifold

Michael G. Scheer,1,∗ Kaiyuan Gu,1 and Biao Lian1
1Department of Physics, Princeton University, Princeton, New Jersey 08544, USA
(Dated: March 14, 2022)

The Bistritzer-MacDonald continuum model (BM model) describes the low-energy moiré bands for twisted bilayer graphene (TBG) at small twist angles. We derive a generalized continuum model for TBG near any commensurate twist angle, which is characterized by a complex inter-layer hopping at commensurate AA stackings (rather than the real hopping in the BM model), a real inter-layer hopping at commensurate AB/BA stackings, and a global energy shift. The complex phase of the AA stacking hopping and the twist angle together define a single angle parameter \( \phi_0 \). We compute the model parameters for the first six distinct commensurate TBG configurations, among which the 38.2° configuration may be within experimentally observable energy scales. We identify the first magic angle for any \( \phi_0 \) at a condition similar to that of the BM model. At this angle, the lowest two moiré bands at charge neutrality become flat (except in the vicinity of the \( \Gamma_M \) point) and retain fragile topology, but lose particle-hole symmetry. We further identify a hyper-magic manifold in the parameter space at \( \phi_0 = \pm \pi/2 \), where seven or more moiré bands around charge neutrality become flat simultaneously. The lowest two moiré flat bands in the hyper-magic manifold have fragile (trivial) topology when close to (far from) the chiral limit with zero AA hopping.

I. Introduction

At certain discrete commensurate twist angles \( \theta_0 \), the hexagonal lattices of two graphene layers align to form a perfectly periodic superlattice [1, 2]. The simplest such commensurate configuration is \( \theta_0 = 0 \) in which two layers of graphene are aligned with no twist. Bistritzer and MacDonald demonstrated that if two layers of graphene are twisted by a small angle relative to this \( \theta_0 = 0 \) configuration, (forming twisted bilayer graphene (TBG)), a moiré superlattice emerges, and the low energy single particle physics can be described by a continuum model [3]. Furthermore, at the so called magic angle, \( \theta \approx 1.05° \), this model predicts that the lowest two moiré bands (i.e. the first conduction and valence bands) become flat simultaneously at charge neutrality. Moreover, it has been shown that the two flat bands carry a fragile topology [4-8], obstructing the construction of maximally localized symmetric Wannier orbitals [9-14]. In this flat band regime, the physics is dominated by interactions, and the low energy approximation from a microscopic tight-binding model. We first show, based on an analysis of the magnitudes of the hopping terms, that the system is approximated by a continuum model of a certain general form. We then use the exact unitary and anti-unitary crystalline symmetries of TBG to constrain the coefficients of this general model. Near commensurate twist angle \( \theta_0 \), we arrive at a TBG continuum model containing four real parameters \( \chi_0, w_0, w_1, w_2 \), which are ultimately determined by the microscopic hopping parameters. We show that \( w_1 \) controls the inter-layer hopping at the commensurate AB and BA stacking configurations and \( w_0 e^{\pm i \chi_0} \) controls the inter-layer hopping at the commensurate AA stacking configuration. \( w_2 \) is simply a global energy shift. When \( \theta_0 = 0 \), the value of \( \chi_0 \) is negligible because of an approx-
inimate mirror symmetry, and we recover the BM model.

In order to determine the model parameters near general commensurate configurations, we consider the geometry of TBG in real space. The key observation is that a small relative rotation $\delta \theta$ of the two graphene layers can be locally approximated by an inter-layer translation [77]. By carefully taking the limit $\delta \theta \to 0$, we derive the model for commensurate twist angle $\theta_0$ and inter-layer displacement $d$ from the model for twist angle $\theta = \theta_0 + \delta \theta$. We then determine the continuum model parameters from a numerical computation of the microscopic tight-binding model (without lattice relaxations [78]) at commensurate angle $\theta_0$ with two values of $d$ corresponding to $AA$ and $AB$ stacking configurations. For the case $\theta_0 = 0$, we recover $w_0 \approx w_1 \approx 110$ meV, $\chi_0 = 0$, $w_2 = 0$ in agreement with the BM model. We additionally provide numerical values of the model parameters for the next five commensurate configurations (in order of the number of atoms per commensurate unit cell). When determining the continuum model parameters, we only use numerical tight-binding results at a single crystal momentum (the commensurate $K$ point) and two $d$ vectors. However, we find that the continuum model matches the tight-binding model with high accuracy for all crystal momenta in the commensurate $K$ valley and all $d$ vectors. It is worth noting that in the first five non-trivial (i.e. $\theta_0 \neq 0$) commensurate configurations, the new parameters $\chi_0$ and $w_2$ are non-negligible. Although we do not consider lattice relaxation or corrugation, we note that these effects can alter the values of the model parameters, but not the general form of the continuum model (assuming these effects preserve the moiré lattice symmetries) [78, 79].

Next, we compute the moiré band structures of TBG with twist angle near the first six commensurate configurations. By both the “tripod model” approximation [3, 80] and accurate numerical computations, we identify the condition for the first magic angle in any nearly commensurate TBG system (Eqs. (65) and (66)). This condition is similar to that of the original BM model. A further simplification of the generic TBG continuum model indicates that the moiré band structure only depends on a single angle variable $\phi_0 = \chi_0 + \frac{w_0}{\tau}$. At the first magic angle, the lowest two bands at charge neutrality in the nearly commensurate TBG model with $\phi_0 \neq 0$ are flat in most of the moiré Brillouin zone except for the vicinity of $\Gamma_M$ point. These bands are no longer particle-hole symmetric, though they do retain fragile topology. For TBG without lattice relaxation, the first magic angle near any nonzero commensurate twist angle $\theta_0$ (e.g. the magic angle $0.004^\circ$ near $\theta_0 \approx 38.2^\circ$) may be too small to be realized experimentally. However, it is possible that spontaneous commensurate atomic structural reconstructions (e.g. charge density wave orders) may enhance the moiré potential and enlarge the magic angles.

Finally, we reveal the existence of a hyper-magic manifold in the parameter space at $\phi_0 = \pm \pi/2$ (Eq. (75)), where no fewer than 7 moiré bands near charge neutrality become extremely flat simultaneously. The hyper-magic manifold persists even when $w_0/w_1 > 1$. In the hyper-magic manifold, the lowest two moiré flat bands at charge neutrality undergo a gap closing transition with remote bands at $w_0/w_1 \approx 0.2$: the two bands have fragile topology when $w_0/w_1 \leq 0.2$ and become topologically trivial when $w_0/w_1 \geq 0.2$. We thus expect that the strongly interacting physics in TBG models in the hyper-magic manifold with $w_0/w_1 \geq 0.2$ may be similar to that of the Hubbard model with trivial bands. In particular, it may host anti-ferromagnetic states.

The rest of this paper is organized as follows. Sec. II derives the generic form of the low energy TBG continuum model near commensuration from the microscopic graphene Hamiltonian. Sec. III further restricts the form of the TBG continuum model by crystalline symmetries, and gives the model parameters for the first six commensurate configurations. In Sec. IV, we discuss the low energy bands (namely the first two conduction and valence bands) of commensurate TBG. Then in Sec. V, we compute the moiré band structure near the commensurate angles with the actual model parameters and give the condition for the first magic angle. In Sec. VI, we further explore the parameter space of the nearly commensurate TBG continuum model, reveal the hyper-magic manifold, and investigate the topology of the moiré bands. Finally, we give a high level discussion in Sec. VII.

II. Derivation of the generic continuum model

A. Microscopic Hamiltonian

The hexagonal crystal structure of monolayer graphene consists of two sublattices $A$ and $B$. We will often make the identifications $A = 1, B = -1$ when using $A$ and $B$ in equations. As shown in Fig. 1(a), the positions of the carbon atoms in sublattice $\alpha$ are given by $r + \tau_\alpha$, for $\alpha \in \{A, B\}$, $r$ in a triangular Bravais lattice $L$, and constant vectors $\tau_\alpha$. It is convenient to choose the primitive vectors $(a_1, a_2)$ for $L$ where $a_1 = a_0 \sqrt{3} \hat{x}$, $a_2 = R_{-\pi/3} a_1$, $a_0 = 1.42 \text{ nm}$ is the inter-atomic distance, and $R_\phi$ de-

![FIG. 1. Illustration of the definitions of quantities in Sec. II A. (a) The graphene lattice and its primitive unit cell. (b) The reciprocal lattice, Brillouin zone, and high-symmetry crystal momenta.](image-url)
notes rotation by angle \( \phi \) about the \( \hat{z} \) axis. Additionally, we choose \( \mathbf{r}_A = a_0 \hat{y} \), \( \mathbf{r}_B = R_{-\pi/3} \mathbf{r}_A \) so that the origin \( \mathbf{0} \) is in the center of a hexagon. We define \( \Omega \) to be the primitive unit cell of \( L \) and \( |\Omega| \) to be its area.

The Bravais lattice \( P \) that is reciprocal to \( L \) has primitive vectors \( (b_1, b_2) \) with \( b_1 = R_{2\pi/3} b_2, b_2 = -4\pi \hat{y}/(3a_0) \) so that \( b_j \cdot a_k = 2\pi \delta_{j,k}. \) Explicitly, the lattices \( L \) and \( P \) are given by

\[
L = \{ n_1 a_1 + n_2 a_2 | n_1, n_2 \in \mathbb{Z} \} \\
P = \{ n_1 b_1 + n_2 b_2 | n_1, n_2 \in \mathbb{Z} \}.
\]

We define the Brillouin zone BZ to be the Wigner-Seitz unit cell of \( P \) and \(|BZ|\) to be its area. Note that \(|\Omega||BZ|\) is block diagonal: the Bloch states \(|k,l,\alpha\rangle\) form a continuous basis for the Hilbert space. However, for convenience we will sometimes use the overcomplete set formed by all Bloch states \(|k,l,\alpha\rangle\) for \( k \in \mathbb{R}^2 \).

We consider a microscopic single-particle Hamiltonian \( H \) with matrix elements

\[
\langle r', l', \alpha'| H | r, l, \alpha \rangle = t_{l/l'}(r + \tau'_{\alpha'} - r - \tau_{\alpha}) - \mu \delta_{\tau', \tau} \delta_{\alpha', \alpha}
\]

(5)

where \( \mu \) is a chemical potential and \( t_{l/l'}: \mathbb{R}^2 \rightarrow \mathbb{R} \) are rotationally symmetric functions (i.e. \( t_{l/l'}(r) \) depends only on \(|r| \)) determining the intra- and inter-layer hopping. We allow the functions \( t_{l/l'}(r) \) to remain unspecified for now. The intra-layer matrix elements are given by

\[
\langle k', l, \alpha'| H | k, l, \alpha \rangle = \langle k', l, \alpha'| k, l, \alpha' \rangle \\
	imes \left( -\mu + \sum_{r \in L + \tau_{\alpha} - \tau_{\alpha}} e^{-i(l_{\alpha}/3) \mathbf{r} \cdot \mathbf{p}} \right)
\]

(6)

(see App. A). If the value of \( \mu \) is chosen appropriately, then for crystal momenta near \( \mathbf{K}_1 = R_{-\pi/2} \mathbf{K} \), this matrix element can be approximated by a Dirac cone

\[
\langle \mathbf{K}_1 + \mathbf{p}', \alpha'| H | \mathbf{K}_1 + \mathbf{p}, \alpha \rangle = \langle \mathbf{K}_1 + \mathbf{p}', \alpha'| H | \mathbf{K}_1 + \mathbf{p}, \alpha \rangle = (\hbar v_F(\sigma_{\alpha}/2) \cdot \mathbf{p})_{\alpha', \alpha} + O(|p|^2) \delta^2(\mathbf{p}' - \mathbf{p})
\]

(7)

Here, \( \sigma_{\alpha} = e^{-i(\phi/2)\sigma_z} (\sigma_x \hat{x} + \sigma_y \hat{y}) e^{i(\phi/2)\sigma_z} \) is a vector of rotated Pauli matrices satisfying

\[
\sigma_{\alpha} \cdot \mathbf{p} = \sigma_{\alpha_0} \cdot (R_0 \mathbf{p}) = \begin{pmatrix} 0 & h.c. \\ e^{i\phi}(p_x + ip_y) & 0 \end{pmatrix}
\]

(8)

and \( v_F \) is the Fermi velocity, which depends on the function \( t_{l/l'}(r) \). See App. B for a derivation of Eq. (7) based on symmetry. The matrix elements for crystal momenta near the other Brillouin zone corners \( R_{\pi/3} \mathbf{K}_1 \) for \( 1 \leq n \leq 5 \) are given by similar Dirac cone Hamiltonians.

The inter-layer matrix elements are given by

\[
\langle k', -l, \alpha'| H | k, l, \alpha \rangle = \sum_{G_{\perp} \in P_{\perp}} \sum_{G_{\parallel} \in P_{\parallel}} \tilde{t}_{-l}(k + G_{\perp}) e^{i\tau_{\alpha}^\perp \cdot G_{\perp}} e^{-i\tau_{\alpha}^\parallel \cdot G_{\parallel}} \delta^2(k + G_{\parallel} - k' - G_{\perp})
\]

(9)

where the hatted functions \( \tilde{t}_{l/l'}(k) \) are the two dimensional Fourier transforms of \( t_{l/l'}(r) \) (see App. A). We see that \( H \) is block diagonal: the Bloch states \(|k', l', \alpha'\rangle\) and \(|k, l, \alpha\rangle\) are in the same Hamiltonian block if and only if

\[
(k' - k) \in P_{\perp} + P_{\parallel}
\]

(10)
where and otherwise 

\[ m, n \] \quad \text{corresponding to the pair \((m, n)\)}.

The commensurate configuration corresponds to the pair \((m, n)\) with \(m > n\) and \(\text{gcd}(m, n) = 1\), in which case the \(L_+\) lattice is invariant under translations by elements of \(L\). Commensurate configurations are those for which \(\delta \theta \neq 0\), by which we mean the twist angle \(\theta\) with \(TBG\) allows us to restrict our attention to configurations for a commensurate configuration.

Commensurate configurations are those for which \(m > n\), and \(\theta\) is invariant under translations by elements of \(L\). Let \(\delta \theta = \theta - 0\) be a commensurate angle, by which we mean the twist angle \(\theta\) for a commensurate configuration.

We show in App. C that the crystalline symmetries of TBG allow us to restrict our attention to configurations with \(\theta \in [0, \pi/3]\). These configurations can be enumerated by a pair of relatively prime integers \(m > n \geq 0\) with

\[ \theta = \cos^{-1}\left(\frac{3m^2 - n^2}{3m^2 + n^2}\right) \]  

(see App. D.1). The commensurate configuration corresponding to the pair \((m, n)\) has 4N atoms per unit cell where the integer \(N \geq 1\) is given in Eq. (D12) as a function of \(m\) and \(n\).

As shown in App. D.3, if \(3|n\) (i.e. 3 divides \(n\)) we have

\[ K_+ - K_-, K'_+ - K'_- \in P_+ + P_+ \]  

and otherwise

\[ K_+ - K'_-, K'_+ - K_- \in P_+ + P_+ \]  

where \(K_l = R_{\pi/2}K\) and \(K'_l = R_{\pi/2}K'\). Additionally, in either case we have

\[ K_+ - K'_+, K_- - K'_- \notin P_+ + P_+. \]

If \(\theta\) is a commensurate angle then so is \(\pi/3 - \theta\), and the Hamiltonians for these two configurations are unitarily equivalent (see App. C). Furthermore, we show in App. D.4 that among the two configurations corresponding to \(\theta\) and \(\pi/3 - \theta\), one must satisfy \(3|n\) while the other does not. As a result, we assume without loss of generality that \(3|n\) and Eq. (12) holds. From here on, we will always assume \(3|n\) unless we explicitly state otherwise. Tab. I lists properties of the first six commensurate configurations in increasing order of \(N\). Fig. 2 illustrates the locations of the atoms in real space for a particular commensurate configuration.

We saw in Eq. (10) that the microscopic Hamiltonian is block diagonal in accordance with the lattice \(P_+ + P_+\). We show in App. D.2 that when the system is commensurate, \(P_+ + P_+\) is the reciprocal lattice of the commensuration superlattice \(L_- \cap L_+\). We see that the block diagonality can be attributed in this case to translation symmetry with respect to the commensuration superlattice. Each Hamiltonian block has a basis consisting of Bloch states with \(N\) non-equivalent crystal momenta in each layer, for a total dimension of \(4N\). As an example, Fig. 3(a) illustrates the crystal momenta involved in the Hamiltonian block containing \(K_+\) and \(K_-\). We show in App. D.5 that \(L_- \cap L_+ = \sqrt{N}L\) and \(P_+ + P_+ = P/\sqrt{N}\), so that the Brillouin zone \(BZ_0\) corresponding to the commensuration superlattice is a regular hexagon.
C. Incommensurate configurations

We now consider an incommensurate twist angle \( \theta \). We show in App. E that in this case \( P_− + P_+ \) is a dense subset of \( \mathbb{R}^2 \). As a result, the block diagonalization of \( H \) given by Eq. (10) cannot be directly used to define a band structure. In this section, we will construct a notion of distance between Bloch states that can be used in place of block diagonalization to analyze \( H \).

We show in App. F that since \( \theta \) is incommensurate, we have \( P_− \cap P_+ = \{0\} \). It follows that for any \( l \in \{+,-\} \) and crystal momentum vectors \( k, k' \) with \( k' - k \in P_− + P_+ \), there are unique vectors \( G_− \in P_−, G_+ \in P_+ \) such that
\[
  k + G_l = k' + G_{−l}. \tag{15}
\]

This pair of vectors \( G_−, G_+ \) determines the inter-layer matrix element in Eq. (9). Since \( t_−(k) \) depends only on \( |k| \), the magnitude of \( \langle k',−l, α'|H|k,l,α \rangle \) depends only on \( |k + G_l| \). We assume that \( t_−(k) \) monotonically decreases with \( |k| \). So that inter-layer matrix elements with large magnitude correspond to small values of \( |k + G_l| \). Similarly, the intra-layer matrix element in Eq. (6) is zero unless \( k' - k \in P_l \). As a result, \( \langle k',l, α'|H|k,l,α \rangle \) is only nonzero when \( k \) and \( k' \) are related as in Eq. (15) with \( |G_{−l}| = 0 \).

With this motivation, we define a function \( d \) that quantifies the magnitude of the matrix elements of \( H \)
\[
d(k, l, k', l') = \begin{cases} 
  \infty & \text{if } k' - k \notin P_− + P_+ \\
  |k + G_l| & \text{if } l' = −l \text{ and Eq. (15)} \\
  |G_{−l}| & \text{if } l' = l \text{ and Eq. (15)}
\end{cases} \tag{16}
\]

We show in App. F that \( d \) satisfies
\begin{enumerate}
  \item \( d(k, l, k, l) = 0 \)
  \item \( d(k, l, k', l') = d(k', l', k, l) \)
  \item \( d(k, l, k'', l''') \leq d(k, l, k', l') + d(k', l', k'', l''') \)
\end{enumerate}
so that \( d \) defines a notion of distance\(^1\) on the set \( \mathbb{R}^2 \times \{+,-\} \). Suppose we define the distance between Bloch states \( |k,l,α\rangle, |k',l',α'\rangle \) to be \( d(k,l,k',l') \). Then by construction, the microscopic Hamiltonian \( H \) described by Eqs. (6) and (9) is local with respect to this notion of distance.

D. Continuum model for incommensurate configurations

We now take
\[
  \theta = \theta_0 + \delta \theta \tag{17}
\]
where \( \theta_0 \) is a commensurate angle (Eq. (11)) and \( \delta \theta \) is small. We assume that \( \theta \) is an incommensurate angle so that the distance function \( d \) from Sec. II C is well defined. We are interested in the single particle physics of \( H \) near the Fermi level at charge neutrality, as this determines the low energy excitations of the many-body Hamiltonian. In this section, we will derive a continuum model that approximates the relevant energies and eigenvectors of \( H \).

We will make use of the following characterization of the distance function \( d \) that applies when \( \theta = \theta_0 + \delta \theta \). Let \( L^0_\alpha = R_{−\delta \theta_0/2}L, P^0 = R_{−\delta \theta_0/2}P \), and recall from Sec. II B that \( L^0_\alpha \cup L^0_\alpha \) is the commensuration superlattice corresponding to twist angle \( \theta_0 \) and \( P^0 + P^0 \) is its reciprocal lattice. Define the set
\[
  Q(k, l, k', l') = −\delta k_0, k' + (k + P^0_0) \cap (k' + P^0_0) \tag{18}
\]
and the operator
\[
  D(\delta \theta) = R_{\delta \theta/2}R_{−\delta \theta/2} = 2 \sin(\delta \theta/2)R_{\pi/2}. \tag{19}
\]

Let \( k \in \mathbb{R}^2, l \in \{+,-\}, \) and define \( k_0 = R_{\delta \theta_0/2}k \). Then for any pair \( (k', l') \) with \( d(k, l, k', l') < \infty \), there are unique vectors \( k_0' \in k_0 + P^0_0 + P^0_α \) and \( Q \in Q(k_0, l, k_0', l') \) such that
\[
  k' = R_{−\delta \theta_0/2}k_0' + lD(\delta \theta)Q. \tag{20}
\]

Additionally, we have \( |Q| = d(k, l, k', l') \) so that
\[
  |R_{−\delta \theta_0/2}k' - k_0'| = 2|\sin(\delta \theta/2)|d(k, l, k', l'). \tag{21}
\]

Conversely, if \( k' \) is given by Eq. (20) for some \( k_0' \in k_0 + P^0_0 + P^0_α \) and \( Q \in Q(k_0, l, k_0', l') \) then \( d(k, l, k', l') = |Q| \). These claims are proved in App. G.

Since monolayer graphene has Dirac cones at the \( K \) and \( K' \) points (i.e. graphene has two valleys), the single particle physics of \( H \) near the Fermi level at charge neutrality is dominated by Bloch states with crystal momenta near \( K \) or \( K' \). Consider two momenta \( k = K_l, k' = K'_l \) from opposite graphene valleys. Then \( k_0 = K_l^0 \) and \( R_{−\delta \theta_0/2}k' = K_l^0 \) where \( K_l^0 \) and \( K_l^0 = R_{−\delta \theta_0/2}K_l \). By Eqs. (12) and (14), \( K_l^0 \notin K_l^0 + P^0_0 + P^0_α \) so there is some minimal value \( \kappa > 0 \) taken by the quantity \( |K_l^0 - k_0'| \) for \( k_0' \in k_0 + P^0_0 + P^0_α \). By Eq. (21),
\[
  d(K_l,l,K'_l, l') \geq \frac{\kappa}{2|\sin(\delta \theta/2)|} \tag{22}
\]
which diverges as \( \delta \theta \to 0 \). This implies that for small \( \delta \theta \), the spectrum of \( H \) splits into two nearly uncoupled valleys corresponding to \( K \) and \( K' \). We will neglect inter-valley coupling and focus on the \( K \) valley, noting that time-reversal symmetry interchanges the valleys (see App. I).

For any \( q > 0 \), define \( U(k, l, q) \) to be the subspace generated by all Bloch states \( |k', l', α'\rangle \) with \( d(k, l, k', l') < q \), and note that \( U(k, l, q) \) is finite dimensional. To compute the eigenstates and energies of \( H \) in the \( K \) valley, we consider the projection of \( H \) into \( U(K_l + p, l, q) \) for a small

\(^1\) Technically, \( d \) is not a metric because it assumes the value \( \infty \) and \( d(k, l, k', l') = 0 \) whenever \( l' = −l, k' \in P_− \) or \( l' = l, k' - k \in P_l \). Nonetheless, it is useful to think of \( d \) as a distance function.
vector $\mathbf{p}$ and a large value $q$. Let $B_{l,q}$ be the set of pairs $(\mathbf{k}^\prime, \mathbf{l}^\prime)$ such that $\mathbf{k}^\prime$ is given by Eq. (20) with $\mathbf{k} = \mathbf{K}_l$, $\mathbf{k}_0^\prime \in \text{BZ}_l^0 = R_{-\nu} \mathbf{b}_0 / 2 \text{BZ}$, and $|Q| < q$. Then for all vectors $\mathbf{p}$ small enough, the set of Bloch states $|\mathbf{k}^\prime + \mathbf{p}, \mathbf{l}^\prime, \alpha^\prime \rangle$ with $(\mathbf{k}^\prime, \mathbf{l}^\prime) \in B_{l,q}$ forms a basis for $U(\mathbf{K}_l + \mathbf{p}, l, q)$. The set $B_{l,q}$ is illustrated in Fig. 3(b).

Recall from Sec. II B that we can write $L_0^\perp \cap L_0^\perp = \sqrt{N} L$ and $P_0^0 + P_0^+ = P / \sqrt{N}$ where $4N$ is the number of atoms in the primitive unit cell of $L_0^\perp \cap L_0^\perp$. When $N > 1$ and $q$ is large enough, there are elements $(\mathbf{k}^\prime, \mathbf{l}^\prime) \in B_{l,q}$ for which the value of $\mathbf{k}_0^\prime$ is not $\mathbf{K}_l^0$ (e.g. the points shown in Fig. 3(b)). The corresponding Bloch states in $U(\mathbf{K}_l + \mathbf{p}, l, q)$ have expected energies with respect to the intra-layer Hamiltonian due to inter-layer coupling to be $\hat{H}_{\text{inter}} = \int d^2 \mathbf{p} d^2 \mathbf{p} |\mathbf{p}', \mathbf{p} \rangle H_{\text{inter}}(\mathbf{p}', \mathbf{p}) |\mathbf{p} \rangle$ where

\[
\hat{H}_{\text{inter}}(\mathbf{p}', \mathbf{p}) = \sum_{Q \in \Sigma} \left( S_Q^+ 0 \quad 0 \right) \delta^2(\mathbf{p}' - \mathbf{p} - D(\delta \theta) Q) + \sum_{Q \in \Sigma^+} \left( 0 T_Q \quad 0 \right) \delta^2(\mathbf{p}' - \mathbf{p} - D(\delta \theta) Q) + \sum_{Q \in \Sigma^+} \left( 0 0 \right) \delta^2(\mathbf{p}' - \mathbf{p} - D(\delta \theta) Q). \tag{30}
\]

Here, $T_Q$ and $S_Q^\dagger$ denote complex $2 \times 2$ matrices which are functions of $\delta \theta$ and the translation parameter $\mathbf{d}$. Note that since $H_{\text{inter}}$ is Hermitian, we have

\[
T_Q^\dagger = T_{-Q}, \quad (S_Q^\dagger)^\dagger = S_Q. \tag{31}
\]

The full continuum Hamiltonian is given by $\hat{H} = \hat{H}_{\text{intra}} + H_{\text{inter}}$.

We show in App. D 5 that

\[
Q_+ = s \sqrt{N} \mathbf{K} + \sqrt{N} \mathbf{P}, \quad Q_0 = \sqrt{N} \mathbf{P}, \tag{32}
\]

where $s = \pm 1$ is given by Eq. (D55). Furthermore, the elements of $Q_+$ with minimal norm are

\[
Q_1 = s \sqrt{N} \mathbf{K}, \quad Q_2 = R_{2\pi/5} Q_1, \quad Q_3 = R_{4\pi/3} Q_1. \tag{33}
\]

The lattices $Q_+, Q_0$ and the vectors $Q_1, Q_2, Q_3$ are shown in Fig. 4. We now observe that $\hat{H}$ is block diagonal: the states $|\mathbf{p}', \mathbf{l}^\prime, \alpha^\prime \rangle_c$ and $|\mathbf{p}, \mathbf{l}, \alpha \rangle_c$ are in the same Hamiltonian block if and only if

\[
|\mathbf{p}' + \mathbf{l} q_1 \rangle - |\mathbf{p} + l q_1 \rangle \in D(\delta \theta) Q_0 \tag{34}
\]

where

\[
q_j = D(\delta \theta) Q_j \quad \text{for} \quad j = 1, 2, 3. \tag{35}
\]

More explicitly, we have

\[
q_1 = 2 \sin(\delta \theta / 2) / s \sqrt{N} |\mathbf{K}| \hat{y}, \quad q_2 = R_{2\pi/3} q_1, \quad q_3 = R_{4\pi/3} q_1. \tag{36}
\]

We refer to $D(\delta \theta) Q_0$ as the moiré reciprocal lattice and $\mathbf{p} + l q_1$ as the moiré quasi-momentum for $|\mathbf{p}, l, \alpha \rangle_c$. The Wigner-Seitz unit cell of the moiré reciprocal lattice is $\text{BZ}_M = D(\delta \theta) \sqrt{N} \text{BZ}$ and it is called the moiré Brillouin zone. Additionally, we define the high-symmetry moiré quasi-momenta

\[
\mathbf{X}_M = D(\delta \theta) s \sqrt{N} \mathbf{X} \tag{37}
\]
for $X \in \{\Gamma, K, K', M\}$ and note that

$$\Gamma_M = 0, \quad K_M = q_1$$

(38)

and

$$|K_M| = 2|\sin(\delta\theta/2)|\sqrt{N}|K|.$$  

(39)

To further explicate the moiré translation symmetry, we transform to real space. We define states

$$|r, l, \alpha\rangle_c = \frac{1}{2\pi} \int d^2p e^{-ip \cdot r} |p, l, \alpha\rangle_c$$

(40)

which satisfy the normalization condition

$$\langle r', l', \alpha' | r, l, \alpha\rangle_c = \delta_{r, r'} \delta_{l, l'} \delta_{\alpha, \alpha} \delta^2(r' - r).$$

(41)

Defining the row vector of states

$$|r\rangle_c = (|r, +, A\rangle_c | r, +, B\rangle_c | r, -, A\rangle_c | r, -, B\rangle_c),$$

(42)

we can rewrite the Hamiltonian in the form

$$\hat{\mathcal{H}}_{\text{int}} = \int d^2r |r\rangle_c \langle r | \mathcal{H}_{\text{int}}(r) |r\rangle_c, \quad \hat{\mathcal{H}}_{\text{inter}} = \int d^2r |r\rangle_c \langle r | \mathcal{H}_{\text{inter}}(r) |r\rangle_c,$$

where

$$\mathcal{H}_{\text{intra}}(r) = -i\hbar v_F \left( \begin{array}{cc} \sigma_{\theta/2} \cdot \nabla & 0 \\ 0 & \sigma_{-\theta/2} \cdot \nabla \end{array} \right)$$

$$\mathcal{H}_{\text{inter}}(r) = \left( \begin{array}{cc} S^+(r) & T(r) \\ T^+(r) & S^-(r) \end{array} \right)$$

(43)

and

$$T(r) = \sum_{Q \in \mathcal{Q}_+} T_Q e^{i\pi D(\delta\theta)Q}$$

$$S^l(r) = \sum_{Q \in \mathcal{Q}_0} S_Q^l e^{i\pi D(\delta\theta)Q}$$

(44)

We interpret $\hat{\mathcal{H}}$ as the Hamiltonian for a system of Dirac electrons moving through the spatially varying potentials $T(r)$, $S^+(r)$, and $S^-(r)$. Note that these potentials are periodic (up to a phase) with respect to the moiré superlattice $D(\delta\theta)^{-1}L/\sqrt{N}$ which is reciprocal to $D(\delta\theta)\mathcal{Q}_0$.

E. Continuum model for commensurate configurations

As in Sec. II D we take $\theta = \theta_0 + \delta\theta$ where $\theta_0$ is a commensurate twist angle, $\delta\theta$ is small, and $\theta$ is an incommensurate angle. Since the microscopic Hamiltonian is continuous with respect to twist angle, we can take the limit $\delta\theta \to 0$ to derive a continuum model for the commensurate configuration with twist angle $\theta_0$.

In this section, we use $T_Q(\delta\theta, d)$, $S_Q(\delta\theta, d)$, $T(r, \delta\theta, d)$, and $S^l(r, \delta\theta, d)$, to denote the $T_Q$ and $S_Q$ matrices and the $T(r)$ and $S^l(r)$ potentials with twist angle $\theta = \theta_0 + \delta\theta$ and translation vector $d$. To determine the correct definition of $T_Q(0, d)$, note that

$$R_{-i\delta\theta/2}r = r - i\delta\theta R_{x/2}r/2 + O(\delta\theta^2) = r - iD(\delta\theta)r/2 + O(\delta\theta^2).$$

(45)

This implies that the pattern of atoms near position $r$ with $\theta = \theta_0 + \delta\theta$ and $d = 0$ is the same to first order in $\delta\theta$ as the pattern with $\theta = \theta_0$ and

$$d = D(\delta\theta)r = 2\sin(\delta\theta/2)R_{x/2}r.$$  

(46)

Taking into account the phase shift accrued by the continuum momentum states when the translation vector $d$ is changed (see App. H), we must then have

$$e^{i\cos(\theta/2)K \cdot \delta\theta}T(r, \delta\theta, 0) = T(r, 0, D(\delta\theta)r) + O(\delta\theta^2)$$

(47)

and so

$$e^{i\cos(\theta/2)K \cdot \delta\theta} \sum_{Q \in \mathcal{Q}_+} T_Q(\delta\theta, 0)e^{i\pi D(\delta\theta)Q}$$

$$= \sum_{Q \in \mathcal{Q}_+} T_Q(0, D(\delta\theta)r) + O(\delta\theta^2).$$

(48)

Taking $r = D(\delta\theta)^{-1}d$ and then taking the limit as $\delta\theta \to 0$ with $d$ fixed, we find

$$\sum_{Q \in \mathcal{Q}_+} T_Q(0, 0)e^{id \cdot (\cos(\theta_0/2)K - Q)} = \sum_{Q \in \mathcal{Q}_+} T_Q(0, d).$$

(49)

A similar calculation shows

$$\sum_{Q \in \mathcal{Q}_0} S^l_Q(0, 0)e^{id \cdot (\cos(\theta_0/2)K - Q)} = \sum_{Q \in \mathcal{Q}_0} S^l_Q(0, d).$$

(50)

Taking $\delta\theta \to 0$ in Eq. (30) then gives

$$\mathcal{H}_{\text{inter}}(p', p) = \mathcal{H}_{\text{inter}}(p', p, 0) \delta^2(p' - p)$$

where

$$\mathcal{H}_{\text{inter}} = \begin{pmatrix} S^+_0(d) & T_0(d) \\ T_0^*(d) & S^-_0(d) \end{pmatrix}.$$

(51)
and

\[ T_0(\vec{d}) = \sum_{\vec{Q} \in \mathbb{Q}} T_{\vec{Q}}(0,0) e^{i\vec{d} \cdot (\cos(\theta_0/2) \vec{K} - \vec{Q})} \]

\[ S_0^i(\vec{d}) = \sum_{\vec{Q} \in \mathbb{Q}^i} \tilde{S}_{\vec{Q}}(0,0) e^{i\vec{d} \cdot (\cos(\theta_0/2) \vec{K} - \vec{Q})}. \]  

(52)

We see that in the commensurate case, the continuum Hamiltonian describes four energy bands, approximating the bands nearest the Fermi level at charge neutrality.

Note that \( T_0(\vec{d}) \) and \( S_0^i(\vec{d}) \) are periodic (up to a phase) with respect to the lattice \( L^0_0 + L^0_+ = L/\sqrt{N} \) which is reciprocal to \( \mathbb{Q}_0 \) (see Apps. D.2 and D.5). As a result, for \( \theta = \theta_0 \) the continuum Hamiltonian \( \tilde{H} \) is periodic in \( \vec{d} \) (up to unitary equivalence) with respect to \( L^0_0 + L^0_+ \). It is worthwhile to note that the microscopic Hamiltonian \( H \) has the exact same periodicity in \( \vec{d} \) (see App. C).

III. Symmetry constraints and model parameters

We now consider the constraints that can be put on the TBG continuum model at twist angle \( \theta = \theta_0 + \delta \theta \) based on the symmetries of TBG, and explicitly determine the parameters of the TBG continuum model near various commensurate angles.

Note that the continuum model is fully determined by the \( T_{\vec{Q}} \) and \( S_{\vec{Q}}^i \) matrices with \( \vec{d} = \vec{0} \) in both the commensurate (\( \delta \theta = 0 \)) and incommensurate (\( \delta \theta \neq 0 \)) cases. We therefore make the assumption that \( \vec{d} = \vec{0} \) throughout this section. For \( \delta \theta \neq 0 \), the valley preserving symmetries of the microscopic Hamiltonian \( H \) are generated by the unitary operators \( C_{3z} \) (rotation by \( 2\pi/3 \) about \( \hat{z} \)), \( C_{2x} \) (rotation by \( \pi \) about \( \hat{x} \)), and the anti-unitary operator \( C_{2z} T \) (time-reversal followed by rotation by \( \pi \) about \( \hat{z} \)). The representations of these symmetry operators on the \( |k, l, \alpha \rangle \) and \( |p, l, \alpha \rangle \) states are given in App. I.

We require that \( \tilde{H} \) commutes with these symmetry operators. \( \tilde{H}_{\text{intra}} \) commutes with the symmetry operators identically so we need only consider \( \tilde{H}_{\text{inter}} \). Assuming \( \delta \theta \neq 0 \), the symmetry constraint \([C_{3z}, \tilde{H}_{\text{inter}}] = 0\) is equivalent to

\[ \sigma_x T_{\vec{Q}} \sigma_x = T_{\vec{Q}}, \quad \sigma_y S_{\vec{Q}} \sigma_y = S_{\vec{Q}}^i \]  

(53)

\[ [C_{3z}, \tilde{H}_{\text{inter}}] = 0 \] is equivalent to

\[ e^{i(2\pi/3)\sigma_z} T_{\vec{Q}} e^{-i(2\pi/3)\sigma_z} = T_{\vec{Q}+e/3} \]

\[ e^{i(2\pi/3)\sigma_z} S_{\vec{Q}}^i e^{-i(2\pi/3)\sigma_z} = S_{\vec{Q}+e/3}^i \]  

(54)

and \([C_{2x}, \tilde{H}_{\text{inter}}] = 0\) is equivalent to

\[ \sigma_x T_{\vec{Q}} \sigma_x = T_{\vec{Q}+\vec{e}}, \quad \sigma_x S_{\vec{Q}} \sigma_x = S_{\vec{Q}+\vec{e}}^i \]  

(55)

where we use the notation \( \vec{M} \) for the complex conjugate of a matrix \( M \). By continuity, these equations also hold for \( \delta \theta = 0 \).

Since \( \tilde{t}_- (\vec{k}) \) monotonically decreases with \( |\vec{k}| \), we expect that the magnitudes of \( T_{\vec{Q}} \) and \( S_{\vec{Q}} \) decay rapidly with \( |\vec{Q}| \). We therefore neglect \( T_{\vec{Q}} \) and \( S_{\vec{Q}}^i \) for all \( \vec{Q} \) with non-minimal norm. Recall that the elements of \( \mathbb{Q}_+ \) of minimal norm are \( \mathbb{Q}_1, \mathbb{Q}_2, \mathbb{Q}_3 \) which are given in Eq. (33). The elements of \( \mathbb{Q}_- \) with minimal norm are \( -\mathbb{Q}_1, -\mathbb{Q}_2, -\mathbb{Q}_3 \), and the only element of \( \mathbb{Q}_0 \) of minimal norm is \( \vec{0} \). See Fig. 4 for an illustration of the \( \mathbb{Q}_1, \mathbb{Q}_2, \mathbb{Q}_3 \) vectors.

By Eq. (31), it suffices to determine the matrices \( T_{\mathbb{Q}_1}, T_{\mathbb{Q}_2}, T_{\mathbb{Q}_3}, S_{\mathbb{Q}_1}, S_{\mathbb{Q}_2}, S_{\mathbb{Q}_3} \) which correspond to minimal norm momenta. By expanding these matrices in the Pauli basis and applying Eqs. (53) to (55) we find

\[ T_{\mathbb{Q}_1} = w_0 e^{i\chi_0 \sigma_z} + w_1 (\sigma_x \cos \zeta_j + \sigma_y \sin \zeta_j), \]

\[ S_{\mathbb{Q}_1} = S_{\mathbb{Q}_2} = w_2 \sigma_0 \]  

(56)

for real model parameters \( \chi_0, w_0, w_1, w_2 \) with \( w_0 \geq 0 \) and \( \chi_0 \in [0, 2\pi) \). Here, we have used \( \zeta_j = \frac{2\pi(j-1)}{3} (j = 1, 2, 3) \) and \( \sigma_0 \) is the \( 2 \times 2 \) identity matrix. Note that the model parameters \( \chi_0, w_1, w_2 \) depend on \( \theta_0 \) and \( \delta \theta \) but not on \( \vec{d} \).

In the special case \( \theta = 0 \) (i.e. no twist) there is an additional valley preserving unitary mirror symmetry \( M_y \) (reflection across the \( \vec{xz} \) plane). The symmetry constraint \([M_y, \tilde{H}_{\text{inter}}] = 0\) is equivalent to

\[ \sum_{\vec{Q} \in \mathbb{Q}_+} [T_{\vec{Q}}, \sigma_z] = \sum_{\vec{Q} \in \mathbb{Q}_0} [S_{\vec{Q}}, \sigma_z] = 0 \]  

(57)

(see App. I). When \( \theta = 0 \), Eq. (57) implies \( \chi_0 = 0 \). Therefore, if the twist angle is near \( 0 \) (i.e. \( \theta_0 = 0, \delta \theta \approx 0 \)) one will find \( \chi_0 \approx 0 \) because of the approximate \( M_y \) symmetry. This agrees with the Bistritzer-Macdonald model for small angle TBG.

In App. J, we show that when \( \delta \theta = 0 \), the model parameters can be determined from numerical computations of the Hamiltonian block containing \( K_{\pm} \) using Eqs. (6) and (9). Additionally, Apps. D.6 and J show that the \( \chi_0, w_0, w_2 \) parameters determine the band structure of \( AA \) stacked commensurate configurations, while the \( w_1, w_2 \) parameters determine the band structure of \( AB \) and \( BA \) stacked commensurate configurations. For numerical computations, we choose the \( t_{\pm}(r) \) functions in Eq. (5) to be those used in Refs. [77, 78, 82] and described in App. K. Tab. I shows approximate values of the model parameters derived from these functions for the first six commensurate configurations in order of the number of atoms per unit cell. Tab. II in App. J lists these parameters with more significant figures. Appendix Fig. 12 shows that the continuum models with parameters in Tab. II are accurate low energy approximations of the microscopic Hamiltonian for all \( \vec{d} \) vectors. Additionally, Appendix Fig. 13 compares the band structures for each commensurate configuration in Tab. II with the band structure derived from the microscopic Hamiltonian, and we see very good agreement. We note that we
do not include any lattice relaxation or corrugation effects here in the microscopic model, and that such effects may alter the true model parameters.

| $(m,n)$ | $\theta_0$ | $\chi_0$ | $(w_0, w_1)$ | $w_2$ |
|---------|------------|----------|--------------|------|
| (1, 0)  | $0^\circ$  | 1        | 0.00$^\circ$ | (113, 113)meV | 0.0meV |
| (5, 3)  | 38.2$^\circ$ | 7        | $-3.10^2$   | (959, 1050)meV | $-4.44$meV |
| (7, 3)  | 27.8$^\circ$ | 13       | $-1$        | (5.50, 3.62)meV | $-4.43$meV |
| (4, 3)  | 46.8$^\circ$ | 19       | $-0.99^4$   | (33.2, 33.2)meV | $-4.32$meV |
| (11, 3) | 17.9$^\circ$ | 31       | 1.24$^2$    | (653, 653)meV  | $-4.43$meV |
| (11, 9) | 50.6$^\circ$ | 37       | $-0.86^2$   | (1300, 1300)meV | $-4.03$meV |

TABLE I. Numerically determined model parameters reported with three significant figures. For the more accurate parameters used in Figs. 5 to 7 and 12 to 14, see Tab. II in App. J.

IV. Commensurate models: band structures

By Eqs. (28), (51), (52) and (56), the continuum model corresponding to commensurate twist angle $\theta_0$ and translation vector $\mathbf{d}$ is $H = \int d^2\mathbf{p}\chi_0 \mathcal{H}_0(\mathbf{p})\chi_0^\dagger(\mathbf{p})$, where the explicit Hamiltonian matrix is

$$\mathcal{H}_0(\mathbf{p}) = w_2 I + \left(\begin{array}{c} \hbar v_F \sigma_{\theta_0/2} \cdot \mathbf{p} & T_0(\mathbf{d}) \\ T_0^\dagger(\mathbf{d}) & -\hbar v_F \sigma_{-\theta_0/2} \cdot \mathbf{p} \end{array}\right) \tag{58}$$

$$T_0(\mathbf{d}) = \sum_{j=1}^3 \mathbf{Q}_j e^{i \mathbf{d} \cdot (\cos(\theta_0/2) \mathbf{K} - \mathbf{Q}_j)} \tag{59}$$

the matrices $\mathbf{Q}_j$ are given in Eq. (56), and $I$ is the $4 \times 4$ identity matrix. Recall that $\sigma_\theta$ is the Pauli matrix vector defined in Eq. (8), $\mathbf{Q}_j$ is defined in Eq. (33), and the momentum space basis $|\mathbf{p}\rangle_e$ is defined in Eq. (29). Using Eqs. (43) and (44) we can also describe this model in real space as $\tilde{H} = \int d^2\mathbf{r} |\mathbf{r}\rangle_e \mathcal{H}_0(\mathbf{r})|\mathbf{r}\rangle_e^\dagger$, where the Hamiltonian matrix takes the form

$$\mathcal{H}_0(\mathbf{r}) = w_2 I + \left(\begin{array}{c} -i \hbar v_F \sigma_{\theta_0/2} \cdot \nabla & T_0(\mathbf{d}) \\ T_0^\dagger(\mathbf{d}) & i \hbar v_F \sigma_{-\theta_0/2} \cdot \nabla \end{array}\right) \tag{60}$$

and the real space basis $|\mathbf{r}\rangle_e$ is defined in Eq. (42).

Fig. 5 shows the low energy band structures of the model in Eqs. (58) and (59) at commensurate angles $\theta_0 = 0$ (untwisted, for which $(m,n) = (1,0)$) and $\theta_0 \approx 38.2^\circ$ (for which $(m,n) = (5,3)$). For both configurations, we show three translation vectors $\mathbf{d}$, and use the parameters in Tab. II. Similar band structures for the other commensurate configurations in Tab. II are shown in Appendix Fig. 13. We compare the band structures of untwisted bilayer graphene and commensurate TBG as follows:

(i) At $AA$ stacking where $\mathbf{d} = 0$. In this case, untwisted bilayer graphene is gapless at momentum $|\mathbf{p}| = |\mathbf{p}_0| = 3|w_0|/(\hbar v_F)$ at charge neutrality (Fig. 5(a)). In contrast, commensurate TBG develops a gap at $|\mathbf{p}| = (m,n) = (1,0)$ ($\theta_0 = 0^\circ$)

(ii) At $BB$ stacking where $\mathbf{d} = \frac{s}{\sqrt{N}}a_0\hat{y}$ (recall that $s = \pm 1$ in Eq. (32)). In this case, both untwisted (Bernal) bilayer graphene (Fig. 5(c)) and commensurate TBG (Fig. 5(d)) have gapless quadratic Dirac band touchings [83] at charge neutrality.

(iii) At generic asymmetric stackings, for instance, $\mathbf{d} = \frac{s}{\sqrt{N}}a_0\hat{x}$. Untwisted bilayer graphene remains gapless (Fig. 5(e)). In contrast, commensurate TBG has a tilted band gap at charge neutrality (Fig. 5(f)), but there may
not be an indirect gap.

Although the above observations are made at exactly commensurate angles, they may also hold for local measurements (e.g. scanning tunneling microscopy (STM) tunneling experiments) near the corresponding stackings if the angle $\theta$ is close enough to a commensurate angle $\theta_0$. In particular, when $\theta_0$ is significantly far from zero, one expects to observe a local charge neutrality gap at AA stacking positions (e.g. a 1.6 meV gap at $\theta_0 \approx 38.2^\circ$). However, we note that the local charge neutrality at AA stacking is generally different from the global charge neutrality of an incommensurate angle, due to local charge transfers between AA stacking regions and AB stacking regions. This can be seen in Fig. 7(b), by noting that the moiré bands at global charge neutrality are close to the conduction band energy at AA stacking in Fig. 5(b).

V. Continuum models near commensuration: moiré band structures and magic angles

The continuum model corresponding to twist angle $\theta = \theta_0 + \delta \theta$ and translation vector $d = 0$ is described by Eqs. (28), (30) and (56). Note that when $\delta \theta \neq 0$, the microscopic Hamiltonians for different choices of translation vector $d$ differ only by a unitary transformation (see App. C). In this section, we summarize the continuum model Hamiltonian and investigate its moiré band structures and magic angles using the parameters determined in Sec. III.

Since $\delta \theta$ is small, we approximate the rotation angles $\pm \theta_0/2$ of the Dirac cones in Eq. (28) by $\pm \theta_0/2$. This is a common approximation in the literature [3]. Additionally, we approximate the $\chi_0, w_0, w_1, w_2$ parameters by their values at angle $\theta_0$ (i.e. with $\delta \theta = 0$), which can be determined using the method described in Sec. III. The continuum model then becomes $\hat{H} = \int d^2p d^2p' \langle \sigma \rangle_e \hat{H}(p', p) \langle \sigma \rangle_e$, where the Hamiltonian matrix

$$\hat{H}(p', p) = \begin{pmatrix} p_0 & \sigma_{-\theta_0/2} \cdot p \\ p_0 & 0 \end{pmatrix} \delta^2(p' - p)$$

$$+ \frac{\hbar v_F}{2} \begin{pmatrix} 0 & \sigma_{\theta_0/2} \cdot p \\ 0 & 0 \end{pmatrix} \delta^2(p' - p)$$

$$+ \sum_{j=1}^3 \begin{pmatrix} 0 & T_q_j \\ 0 & 0 \end{pmatrix} \delta^2(p' - p - q_j)$$

$$+ \sum_{j=1}^3 \begin{pmatrix} 0 & T_q_j \\ 0 & 0 \end{pmatrix} \delta^2(p' - p + q_j),$$

and the matrices $T_q_j$ are defined in Eq. (56). Recall that $\sigma_\phi$ is the Pauli matrix vector defined in Eq. (8), $q_j$ is defined in Eq. (35), and the momentum space basis $|\sigma\rangle_e$ is defined in Eq. (29). Note that $w_2$ is solely a constant energy shift.

Using Eqs. (43) and (44) we can also describe this model in real space by $\hat{H} = \int d^2r |r\rangle \langle r| \hat{H}(r) \langle r|$, where

$$\hat{H}(r) = w_2 I + \begin{pmatrix} -i \hbar v_F \sigma_{\theta_0/2} \cdot \nabla \\ T(r) \end{pmatrix}$$

$$T(r) = \sum_{j=1}^3 T_q_j e^{ir \cdot q_j},$$

and the real space basis $|r\rangle_e$ is defined in Eq. (42).

Following [3, 12], we introduce the dimensionless parameter

$$\alpha = \frac{w_1}{\hbar v_F |K_M|} = \frac{|w_1|}{2|\sin(\delta \theta/2)| \hbar v_F \sqrt{N}|K|^3}.$$
we conclude that the first magic angle occurs at remote bands \([80]\), and this is also true here. By Eq. (64),

\[ w_c \text{ typically requires} \]

\[ \theta \text{ point is generically nonzero when} \]

\[ \theta \text{ is the number of atoms in each commen-} \]

\[ \text{surate unit cell at twist angle} \theta_0. \text{ Note that} \alpha^{-1} \propto |\delta \theta| \text{ when} \delta \theta \text{ is small.} \]

\[ \text{As a first step in the search for magic angles, we cut off the continuum model in Eq. (62) to a subspace of four quasi-momenta,} \mathbf{p} \text{ and} \mathbf{p} - \mathbf{q}_j \ (j = 1, 2, 3). \text{ This truncation is known as the tripod model approximation} \]

\[ \text{[3, 80]} \text{ and it yields an approximate} \mathbf{k} \cdot \mathbf{p} \text{ model at the} \mathbf{K}_M \]

\[ \text{point at charge neutrality. Generically, the lowest bands of this model have a Dirac fermion spectrum with Fermi velocity} v_M. \text{ In this tripod model approximation, it can be shown (see App. M) that the velocity} v_M \text{ reaches its minimum (which is generically nonzero unless} \theta_0 = 0 \text{) near} \]

\[ \alpha^{-1} \approx \sqrt{3}, \]

\[ \text{given that the energy} E \text{ at the} \mathbf{K}_M \text{ point satisfies} \]

\[ \frac{E - w_2}{\hbar v_F K_M} \ll 1. \text{ Note that the energy} E - w_2 \text{ at the} \mathbf{K}_M \]

\[ \text{point is generically nonzero when} \theta_0 \text{ is nonzero. It is also} \]

\[ \text{known that the magic angle condition Eq. (65) generi-} \]

\[ \text{cally requires} w_0 \leq |w_1| \text{ to avoid hybridization with the} \]

\[ \text{remote bands [80], and this is also true here. By Eq. (64),} \]

\[ \text{we conclude that the first magic angle occurs at} \]

\[ \delta \theta = \delta \theta_{\text{magic}} \approx \pm \frac{\sqrt{3}w_1}{\hbar v_F \sqrt{N\mathbf{K}}} \] .

\[ \text{The tripod model approximation, however, does not give the higher (i.e. second, third, etc.) magic angles.} \]

\[ \text{Fig. 6(a) and (b) show numerical results of Dirac velocities} v_M \text{ and the bandwidth of the lowest two moiré bands at charge neutrality, near commensurate angles} \]

\[ \theta_0 = 0^\circ \ (\text{with} \ (m, n) = (1, 0)) \text{ and} \theta_0 \approx 38.2^\circ \ (\text{with} \ (m, n) = (5, 3)), \text{ respectively. The blue curves show} \frac{v_M}{v_F} \text{ computed from the tripod model, and have a minimum around} \]

\[ \text{Eq. (66). The red curves show the accurate} \frac{v_M}{v_F} \text{ computed by keeping 632 moiré bands. In both cases, the} \]

\[ \text{value of} v_M/v_F \text{ is computed by numerical differen-} \]

\[ \text{tialization in the} \mathbf{q}_F \text{ direction at} \mathbf{K}_M. \text{ Intriguingly, at} \theta_0 \approx 38.2^\circ, \text{ the accurate Fermi velocity} v_M \text{ at the first magic angle} \]

\[ \delta \theta_{\text{magic}} \text{ is almost zero and much smaller than that found in the tripod model. The black curves show the total bandwidth (in units of} \hbar v_F |\mathbf{K}_M| \text{ of the lowest two bands at charge neutrality. From the accurate} \frac{v_M}{v_F} \text{ (red) and} \]

\[ \text{bandwidth (black) curves, we clearly see the first magic angle around} \]

\[ \text{Eq. (66). There are higher (smaller) magic angles near} \theta_0 \approx 38.2^\circ \text{ as well, where the lowest two bands become flat.} \]

\[ \text{Fig. 7(a) and (b) show the moiré band structures at the first magic angle} \delta \theta = \delta \theta_{\text{magic}} \text{ near commensurate angles} \]

\[ \theta_0 = 0^\circ \text{ and} \theta_0 \approx 38.2^\circ, \text{ respectively. The band structure with} \theta_0 = 0^\circ \text{ shows the usual magic angle moiré bands of small angle TBG studied in [3]. At} \theta_0 \approx 38.2^\circ, \]

\[ \text{the band structure is clearly not symmetric across the} \]

\[ \text{Fermi level, indicating the absence of both particle-hole sym-} \]

\[ \text{metry} P \text{ [5, 45, 84] and chiral symmetry} C_{12} \text{ (see definitions in App. L). The lowest two moiré bands at charge neutrality are still approximately flat near the} \]

\[ \mathbf{K}_M \text{ and} \mathbf{K}'_M \text{ points, and are energetically shifted close to a remote conduction band (Fig. 7(b)). The two bands are not quite flat near the} \Gamma_M \text{ points, as a result of hybridization with the remote conduction bands. Moiré band structures at the first magic angle in Eq. (66) near the other commensurate configurations listed in Tab. I are shown in Fig. 14. Additionally, other example moiré band structures near the first magic angle can be found in Fig. 9 and App. N.} \]

\[ \text{Tab. II shows the values of} \delta \theta_{\text{magic}} \text{ for the first six commensurate configurations. Due to the small magnitude of} \]

\[ w_0, w_1 \text{ for nonzero commensurate angles, the correspond-} \]

\[ \text{ing values of} \delta \theta_{\text{magic}} \text{ are so small that they likely cannot} \]

\[ \text{be achieved experimentally. However, we note the possi-} \]

\[ \text{bility that atomic structural reconstructions (e.g. charge density wave orders) may occur in large twist angle TBG} \]

\[ \text{(modulating between} AA \text{ and} AB \text{ stackings) and enhance the effective inter-layer hopping} w_0, w_1. \text{ Provided the} \]

\[ \text{structural reconstructions do not break the symmetries of the moiré superlattice (translation,} C_{3z}, C_{2z} T, C_{2z}, \text{ the form of effective continuum model will not change, and we may arrive at a larger first magic angle in nearly commensurate TBG.} \]
VI. Flat bands in the continuum model parameter space: the hyper-magic manifold

Regarding the possibility that the actual model parameters may change due to atomic structural reconstruction, lattice relaxation, and corrugation, in this section, we investigate the band structure of the TBG continuum model near commensuration in Eq. (62) with arbitrary parameters. Remarkably, we reveal the existence of a hyper-magic manifold in the parameter space, where 7 or more moiré bands become extremely flat simultaneously.

A. Model simplification

We first simplify the continuum model in Eq. (62) by applying a unitary transformation of the basis from \( |p\rangle_c \) to \( |p\rangle'_c = |p\rangle_c U_{\theta_0} \), where

\[
U_{\theta_0} = \left( \begin{array}{cc} e^{i(\theta_0/4)\sigma_z} & 0 \\ 0 & e^{-i(\theta_0/4)\sigma_z} \end{array} \right). \tag{67}
\]

Such a transformation removes the rotation angles \( \pm \theta_0/2 \) for the Dirac cones, and transforms the Hamiltonian into

\[
\mathcal{H}'(p', p) = w_2 I \delta^2(p' - p) + i \hbar v_F \begin{pmatrix} \sigma \cdot p & 0 \\ 0 & \sigma \cdot p \end{pmatrix} \delta^2(p' - p) + \sum_{j=1}^{3} \left( \begin{array}{c} T_{Q_j}' \\ 0 \end{array} \right) \delta^2(p' - p - q_j) + \sum_{j=1}^{3} \left( \begin{array}{c} 0 \\ T_{Q_j}' \\ 0 \end{array} \right) \delta^2(p' - p + q_j).
\]

Here, \( \sigma = \sigma_x \hat{x} + \sigma_y \hat{y} \) is a vector of Pauli matrices, and

\[
T_{Q_j}' = e^{i(\theta_0/4)\sigma_z} T_{Q_j} e^{i(\theta_0/4)\sigma_z}. \tag{69}
\]

More explicitly,

\[
T_{Q_j}' = w_0 e^{i\phi_0\sigma_z} + w_1 (\sigma_x \cos \zeta_j + \sigma_y \sin \zeta_j), \tag{70}
\]

where \( \zeta_j = \frac{2\pi(j-1)}{3} \) (\( j = 1, 2, 3 \)), and we have defined

\[
\phi_0 = \chi_0 + \frac{\theta_0}{2}. \tag{71}
\]

Therefore, the angles \( \chi_0 \) and \( \theta_0 \) are not independent, and we are left with a single angle variable \( \phi_0 \) in the continuum model of Eq. (68), occurring in the matrices \( T_{Q_j}' \) in Eq. (70). We note that the angle \( \phi_0 \) in Eq. (71) also occurs in the expression of the gap for the commensurate AA stacking configuration in Eq. (61). This can also be understood via the transformation in Eq. (67).

The model can similarly be written in the transformed real space basis \( |r\rangle'_c = |r\rangle_c U_{\theta_0} \). The Hamiltonian then becomes

\[
\mathcal{H}'(r) = w_2 I + \begin{pmatrix} -i \hbar v_F \sigma \cdot \nabla & -i \hbar v_F \sigma \cdot \nabla \\ T'(r) & -i \hbar v_F \sigma \cdot \nabla \end{pmatrix}, \tag{72}
\]

and where we have defined

\[
T'(r) = \sum_{j=1}^{3} T_{Q_j}' e^{i\phi_j q_j} \tag{73}
\]
in terms of the matrices \( T_{Q_j}' \) in Eq. (70).

By the results of App. L, we can assume without loss of generality that \( s = 1 \) (recall that \( s \) affects the direction of \( q_j \), see Eqs. (33) and (35)), and

\[
\phi_0 \in \left[ 0, \frac{\pi}{2} \right], \quad w_0 \geq 0, \quad w_1 \geq 0, \quad \delta \theta \geq 0. \tag{74}
\]

In addition, since \( w_2 \) simply shifts the energy bands globally, we assume \( w_2 = 0 \) hereafter. As shown in App. L, the moiré band structures at angle \( \phi_0 \) and angle \( -\phi_0 \) are particle-hole transformations of each other, while the moiré band structures at angle \( \phi_0 \) and angle \( \pi - \phi_0 \) are equivalent.

We note that in the chiral limit \( w_0 = 0 \) [12], the continuum model in Eq. (68) is independent of the angle \( \phi_0 \). This is revealed as a symmetry of the TBG continuum model in the chiral limit in Ref. [14].

B. Changing \( \phi_0 \) near the first magic angle

We first describe the evolution of the flat bands with respect to \( \phi_0 \) (see Eq. (71)) near the first magic angle, or the so-called first magic manifold [80], given by \( \alpha^{-1} \approx \sqrt{3} \) (see Eq. (65))) and \( 0 \leq w_0/w_1 \leq 1 \).

At \( \phi_0 = 0 \), the lowest two flat bands at the first magic angle \( \alpha^{-1} \approx \sqrt{3} \) at charge neutrality are fixed at zero energy due to a particle-hole symmetry \( P \) [5] (see definition in App. L), and are known to be extremely flat for the entire interval \( w_0/w_1 \in [0, 1] \). This can be seen in the bandwidth plot of Fig. 8(b) at \( \phi_0 = 0 \), where the dark purple line near \( \alpha^{-1} \approx \sqrt{3} \) extends over the entire interval \( w_0/w_1 \in [0, 1] \). Band structure examples can be found in Fig. 7(a) and Fig. 9(a).

For a fixed \( w_0/w_1 \) and near the first magic angle at \( \alpha^{-1} \approx \sqrt{3} \), tuning \( \phi_0 \) away from 0 shifts the two flat bands at charge neutrality away from zero energy (breaking the particle-hole symmetry \( P \)), and gradually increases the bandwidth of the flat bands. As shown in Fig. 8(a), the bandwidth around \( \alpha^{-1} = \sqrt{3} \) increases as \( \phi_0 \) increases from 0 to \( \pi/2 \), but still shows a local minimum near \( \alpha^{-1} \approx \sqrt{3} \) (though the minimizing value of \( \alpha^{-1} \) decreases as \( \phi_0 \) increases). The increasing of the bandwidth is because of the hybridization between the
flat bands and the next remote band near the \( \Gamma_M \) point. This can be seen in Fig. 7(b), Fig. 9(b)-(d), where the red and blue bands are the lowest two bands at charge neutrality. In particular, the lowest two bands at charge neutrality remain rather flat near the \( K_M \) and \( K'_M \) points for small \( \phi_0 \) (see also Appendix Figs. 14 and 15), thus providing a realization of bands flat in the Brillouin zone except in the vicinity of the \( \Gamma_M \) point.

C. The hyper-magic manifold at \( \phi_0 = \pm \pi/2 \)

One may have noticed that in the bandwidth plot Fig. 8(a) (for which \( w_0/w_1 = 0.8 \)), there are three dark spots at \( \phi_0 = \pi/2 \) near \( \alpha^{-1} \approx 0.7 \), \( \alpha^{-1} \approx 0.4 \), and \( \alpha^{-1} \approx 0.3 \), which have extremely small bandwidths for the lowest two bands at charge neutrality. The situation is identical at \( \phi_0 = -\pi/2 \), which is related to \( \phi_0 = \pi/2 \) by a particle-hole transformation \( P \) (see App. L).

To investigate what happens to the flat bands at \( \phi_0 = \pm \pi/2 \), we compute the bandwidth of the lowest two bands at charge neutrality at angle \( \phi_0 = \pi/2 \), as a function of \( \alpha^{-1} \) and \( w_0/w_1 \). The result is given in Fig. 8(c), where we find a small bandwidth manifold around \( \alpha^{-1} \approx 0.7 \), \( \alpha^{-1} \approx 0.4 \) and \( \alpha^{-1} \approx 0.3 \), i.e. the three dark horizontal purple lines, extending from \( w_0/w_1 = 0 \) all the way to the vast parameter space of \( w_0/w_1 > 1 \). Note that the upper two dark lines cross around \( w_0/w_2 \approx 0.2 \) at \( \alpha^{-1} \approx 0.45 \).

Fig. 9(e) and (f) show the moiré band structures at angle \( \phi_0 = \pi/2 \) and \( w_0/w_1 = 0.8 \), for \( \alpha^{-1} = 0.681 \) and \( \alpha^{-1} = 0.427 \), respectively (located at the upper two dark lines in Fig. 8(c)). Surprisingly, in both cases, we find there are several more extremely flat conduction and valence bands in addition to the lowest two bands at charge neutrality. In total, there are simultaneously 7 flat bands in Fig. 9(e), and 9 flat bands in Fig. 9(f)!

A further numerical exploration shows that the existence of multiple flat bands is robust along the three near-horizontal dark purple lines in Fig. 8(e) (see Appendix Fig. 16), except near the crossings of the upper two lines around \( w_0/w_1 \approx 0.2 \) where the bandwidth is slightly higher. We define this new manifold consisting of the three dark purple lines in Fig. 8(c) as the hyper-magic manifold:

\[
\phi_0 = \pm \frac{\pi}{2}, \; \alpha^{-1} \approx 0.69, 0.42 \text{ or } 0.30
\]

(\( \alpha^{-1} \) depends on \( w_0/w_1 \), here we take \( w_0/w_1 \approx 1 \))

\[(\text{Eq. (75))}\]

If one realizes such a system with \( \phi_0 = \pm \pi/2 \) (e.g. near a commensurate configuration with properly chosen \( \theta_0 \) and \( \gamma_0 \) in Eq. (71)), we call the corresponding twist angle \( \delta \theta \) (proportional to \( \alpha^{-1} \) by Eq. (64)) a hyper-magic angle.

We note that the values of \( \alpha^{-1} \) deviate from 0.69, 0.42 and 0.30 when \( w_0/w_1 \) is far from 1: the upper two dark lines cross each other around \( w_0/w_1 \approx 0.2 \), while the lower two dark lines merge together when \( w_0/w_1 > 2 \), as shown in Fig. 8(c). The name “hyper-magic” refers to
FIG. 9. Moiré band structures using the model in Eq. (68) with \( w_0/w_1 = 0.8 \) and \( w_2 = 0 \). The first four band structures correspond to the first magic angle (Eq. (65)) with varying \( \phi_0 \). The last two band structures correspond to the hyper-magic manifold (Eq. (75)). All band structures follow the moiré quasi-momentum trajectory \( \Gamma_M \rightarrow K_M \rightarrow M_M \rightarrow \Gamma_M \rightarrow -M_M \rightarrow -K_M \) (note that \(-K_M\) is equivalent to \(K'_M\)). The lowest two bands at charge neutrality are shown in blue and red while the other bands are shown in black.

the remarkable fact that a single parameter \( \alpha \) simultaneously tunes the flatness of 7 or more bands. In particular, we find the number of flat bands in the hyper-magic manifold generically increases as \( w_0/w_1 \) increases, as shown in Appendix Fig. 16. Around \( w_0/w_1 \approx 2 \), one achieves more than 10 flat bands simultaneously. Additionally, we note that the upper two dark lines of the hyper-magic manifold in the chiral limit \( w_0/w_1 = 0 \) coincide with the second and the third magic angles therein [12], where there are also higher flat bands in addition to the two flat bands at charge neutrality (see Appendix Fig. 16(i) and (j)).

Taking a closer look at the moiré band structure around charge neutrality in the hyper-magic manifold (Fig. 9(e) and (f)), we see groups of 3 connected bands (e.g. the 2nd to 4th valence bands below charge neutrality in Fig. 9(e)) where one of them is extremely flat, with quadratic band touching at the \( \Gamma_M \) point, and Dirac points at the \( K_M, K'_M \) points between the other two bands. We believe each group of such 3 connected bands resemble a those of a tight-binding model on the Kagome lattice [85, 86]. Intriguingly, a band inversion transition occurs along the lowest dark line of the hyper-magic manifold in Fig. 8(c) around \( w_0/w_1 = 0.86 \), below which \( (w_0/w_1 < 0.86) \) the lowest two moiré bands at charge neutrality become part of a group of 3 connected Kagome-like bands (Appendix Fig. 17(d)-(f)). In addition, there are more non-trivial groups of 4 connected bands (e.g. the 2nd to 5th conduction bands above charge neutrality in Fig. 9(f)), containing a flat band at the top and another flat band at the bottom. We leave the investigation of the effective model of such 4 connected bands to future study.

The continuum model in Eq. (68) (with \( w_2 = 0 \)) at \( \phi_0 = \pm \pi/2 \) clearly has neither the particle-hole symmetry \( P \) nor the chiral symmetry \( C \) (see definition in App. L), due to the asymmetry between conduction bands and valence bands. As shown in App. L, the particle-hole transformation \( P \) maps the Hamiltonian \( \hat{H} \) at angle \( \phi_0 \) to \(-\hat{H}\) at angle \(-\phi_0\), while keeping the other parameters invariant. In contrast, the chiral transformation \( C \) maps \( \hat{H} \) at angle \( \phi_0 \) to \(-\hat{H}\) at angle \( \phi_0 - \pi \), while keeping the other parameters invariant. Therefore, the continuum model at angle \( \phi_0 = \pm \pi/2 \) has a combined \( CP \) symmetry:

\[
[CP, \hat{H}] = 0 \quad \text{at} \quad \phi_0 = \pm \frac{\pi}{2}
\]  

No other values of \( \phi_0 \) possess this symmetry unless \( w_0 = 0 \).

D. Band topology

Lastly, we discuss the band topology of the lowest two moiré bands at charge neutrality. It is known that in the small angle TBG continuum model [3], which corresponds to \( \phi_0 = 0 \) here (in Eq. (71)), the lowest two moiré bands carry a fragile topology protected by \( C_{2z,T} \) symmetry, provided the two bands are disconnected with the remote bands [4–8, 87–89]. It is further shown by
\[ \alpha^{-1} = 1.732, \phi_0 = 0, \quad \frac{w_0}{w_1} = 0.8 \]
\[ \alpha^{-1} = 1.689, \phi_0 = \pi/6, \quad \frac{w_0}{w_1} = 0.8 \]
\[ \alpha^{-1} = 1.607, \phi_0 = \pi/2, \quad \frac{w_0}{w_1} = 0.8 \]
\[ \alpha^{-1} = 0.450, \phi_0 = \pi/2, \quad \frac{w_0}{w_1} = 0.1 \]
\[ \alpha^{-1} = 0.681, \phi_0 = \pi/2, \quad \frac{w_0}{w_1} = 0.8 \]
\[ \alpha^{-1} = 0.426, \phi_0 = \pi/2, \quad \frac{w_0}{w_1} = 0.8 \]

Fig. 10. Wilson loop bands for the lowest two moiré bands at charge neutrality, for various parameters. The Wilson loop winding number is 1 if the two bands have fragile topology, and is 0 if the two bands have trivial topology. The parameters for panels (a)-(c), (e), (f) are the same as those in Fig. 9(a), (b) and (d)-(f), respectively.

Ref. [84] that, in the presence of both the \( C_{2z} T \) symmetry and the particle-hole symmetry \( P \) (which is the case when \( \phi_0 = 0 \)), the fragile topology becomes stable.

The fragile topology in the lowest two moiré bands at charge neutrality can be detected by calculating their Wilson loop winding number modulo 2 [5, 84]. Taking the moiré Brillouin zone as a rhombus, we label the quasi-momentum \( p \) by its projections \((p_1, p_2)\) onto the two moiré Brillouin zone edges. One can then define the 2 × 2 Wilson loop operator along a loop [90, 91]

\[
W(p_1) = \lim_{N_p \to \infty} \prod_{j=0}^{N_p-1} u^l \left( p_1, j \frac{2\pi}{N_p} \right) u \left( p_1, (j+1) \frac{2\pi}{N_p} \right),
\]

where \( u(p_1, p_2) \) are the wavefunctions of the two bands, and \( j = N_p \) is identified with \( j = 0 \) (via a sewing matrix, see Refs. [5, 84]). If the two eigenvalues of \( W(p_1) \) are given by \( e^{\pm \lambda_\pm(p_1)} \), one can examine the winding number of the Wilson loop bands \( \lambda_\pm(p_1) \). Fig. 10(a) shows the Wilson loop bands of the lowest two moiré bands at \( \phi_0 = 0 \), \( \alpha^{-1} = 1.732 \) and \( \frac{w_0}{w_1} = 0.8 \) (corresponding to small angle TBG at the first magic angle), which has winding number 1, indicating non-trivial fragile topology. Away from \( \phi_0 = 0 \), TBG no longer has particle-hole symmetry \( P \), so the fragile topology of the lowest two moiré bands may be lost.

We find the fragile topology of the lowest two moiré flat bands at charge neutrality remains robust for any \( \phi_0 \in [0, \pi/2] \) near the first magic angle (first magic manifold [80]) \( \alpha^{-1} \approx \sqrt{3} \), if they are gapped from the remote bands. Two examples of the Wilson loop bands in this regime (with \( \frac{w_0}{w_1} = 0.8 \)) are given in Fig. 10(b) and (c), both having a Wilson loop winding number 1, indicating fragile topology.

The Wilson loop computations around the hyper-magic manifold at \( \phi_0 = \pi/2 \) show that the lowest two moiré flat bands at charge neutrality undergo a transition between fragile topology and trivial topology at \( \frac{w_0}{w_1} \approx 0.2 \) (the precise value depends on \( \alpha^{-1} \) and is here estimated around \( \alpha^{-1} = 0.46 \)), via gap closing with the remote bands. Such a gap closing transition can be seen in Appendix Fig. 17(a)-(c).

On the \( \frac{w_0}{w_1} < 0.2 \) side of the hyper-magic manifold (the dark lines in Fig. 8(c)), namely, close to the chiral limit \( \frac{w_0}{w_1} = 0 \), the lowest two moiré flat bands have fragile topology as expected in the chiral limit [4–8]. Fig. 10(d) shows such an example at \( \alpha^{-1} = 0.450, \frac{w_0}{w_1} = 0.1 \) and \( \phi_0 = \pi/2 \), where the Wilson loop winding number is 1.

On the \( \frac{w_0}{w_1} > 0.2 \) side of the hyper-magic manifold, the lowest two moiré flat bands become topologically trivial. Fig. 10(e) and (f) show the Wilson loop bands in the hyper-magic manifold at \( \frac{w_0}{w_1} = 0.8 \) for \( \alpha^{-1} = 0.681 \) and \( \alpha^{-1} = 0.426 \), respectively, both of which have winding numbers 0. With Dirac points protected by \( C_{2z} T \) symmetry at \( K_M \) and \( K_M \) points, the two lowest flat moiré bands should resemble a honeycomb tight-binding model similar to monolayer graphene.

Intriguingly, the gap closing band topology transition at \( \frac{w_0}{w_1} \approx 0.2 \) is also approximately where the crossing of the two dark lines of the hyper-magic manifold occurs in Fig. 8(c). This can be seen in Fig. 17(b) computed at the crossing point of the hyper-magic manifold, which shows that the lowest two moiré bands touch the remote bands.

VII. Discussion

We have derived an effective low energy continuum model for TBG at angle \( \theta = \theta_0 + \delta \theta \) near generic commensurate angles \( \theta_0 \). The model is characterized by a complex inter-layer hopping amplitude \( w_{0,1}^{\pm \pi/2} \) at commensurate \( AA \) stackings, a real inter-layer hopping amplitude \( w_1 \) at commensurate \( AB/BA \) stackings, and a global energy shift \( w_2 \). The twist angle \( \theta_0 \) and the phase \( \chi_0 \) combine into a single angle parameter \( \phi_0 = \chi_0 + \frac{\theta_0}{2\pi} \) which affects the band structure of the effective continuum model (Eq. (68)). Unless \( \theta_0 = 0 \) (i.e. small angle TBG), \( \phi_0 \) is generically nonzero. Taking the \( \delta \theta \rightarrow 0 \) limit yields a low-energy \( k \cdot p \) model for commensurate TBG, which gives a nonzero charge neutrality gap in the \( AA \) stacking case if \( \phi_0 \neq 0 \)(mod \( \pi \)), and gapless quadratic band touching in the \( AB \) stacking case. For commensurate angle \( \theta_0 \approx 38.2^\circ \), the gap in the \( AA \) stacking case is around 1.6meV and is therefore experimentally detectable. Away from commensurate angles, we find the first magic angle \( \delta \theta_{\text{magic}} \) near a generic commensurate angle \( \theta_0 \) is still approximately given by \( \alpha^{-1} = \sqrt{3} \)
of anti-ferromagnetic states, in contrast to the spin-valley ferromagnetic states in interacting magic angle TBG with \( \phi_0 = 0 \) [44, 45, 57–59].

A practical future question is how to achieve a continuum model with large angle \( \phi_0 \) with sufficiently large energy scales (parameters \( w_0, w_1 \)) to be observable in experiment. Ideally it would be most interesting to approach the hyper-magic manifold at \( \phi_0 = \pm \pi/2 \). The effective hoppings \( w_0 \) and \( w_1 \) at nonzero commensurate angles \( \theta_0 \) (without lattice relaxation) are generically small. For example, \( w_0, w_1 \) at \( \theta_0 \approx 38.2^{\circ} \) are about 1 percent of those at \( \theta_0 = 0^{\circ} \). One idea to enhance \( w_0, w_1 \) is to explore the possibility of atomic interaction induced structural reconstruction (e.g. charge density waves) or lattice relaxation, which may enhance the moiré potential modulation between commensurate AA and AB/BA stackings. In addition, for small twist angles near the untwisted configuration \( \theta_0 = 0 \), breaking the mirror symmetry \( M_y \) (while preserving the other symmetries) would allow \( \chi_0 \) to be nonzero, and thus \( \phi_0 \) nonzero. Thus, strong \( M_y \) breaking perturbations in certain forms may drive small angle TBG into a large \( \phi_0 \) model. It may also be possible to approach this continuum model in a subspace of a model for twisted graphene multilayers near commensuration. We leave these ideas them for future study.

Acknowledgments

We thank Jonah Herzog-Arbeitman for valuable discussions. This work is supported by the Alfred P. Sloan Foundation and the NSF through Princeton University’s Materials Research Science and Engineering Center DMR-2011750.

[1] S. Shallcross, S. Sharma, and O. A. Pankratov, Quantum interference at the twist boundary in graphene, Physical Review Letters 101, 1 (2008).
[2] S. Shallcross, S. Sharma, E. Kandelaki, and O. A. Pankratov, Electronic structure of turbostratic graphene, Physical Review B 81, 10.1103/PhysRevB.81.165105 (2010).
[3] R. Bistritzer and A. H. MacDonald, Moiré bands in twisted double-layer graphene, Proceedings of the National Academy of Sciences of the United States of America 108, 12233 (2011).
[4] H. C. Po, L. Zou, A. Vishwanath, and T. Senthil, Origin of Mott Insulating Behavior and Superconductivity in Twisted Bilayer Graphene, Physical Review X 8, 031089 (2018).
[5] Z. Song, Z. Wang, W. Shi, G. Li, C. Fang, and B. A. Bernevig, All Magic Angles in Twisted Bilayer Graphene are Topological, Physical Review Letters 123, 036401 (2019).
[6] H. C. Po, L. Zou, T. Senthil, and A. Vishwanath, Faithful tight-binding models and fragile topology of magic-angle bilayer graphene, Physical Review B 99, 195455 (2019).
[7] J. Ahn, S. Park, and B.-J. Yang, Failure of Nielsen-Ninomiya Theorem and Fragile Topology in Two-Dimensional Systems with Space-Time Inversion Symmetry: Application to Twisted Bilayer Graphene at Magic Angle, Physical Review X 9, 021013 (2019).
[8] B. Lian, F. Xie, and B. A. Bernevig, Landau level of fragile topology, Phys. Rev. B 102, 041402 (2020).
[9] J. Kang and O. Vafek, Symmetry, Maximally Localized Wannier States, and a Low-Energy Model for Twisted Bilayer Graphene Narrow Bands, Phys. Rev. X 8, 031088 (2018).
[10] M. Koshino, N. F. Q. Yuan, T. Koretsune, M. Ochi, K. Kuroki, and L. Fu, Maximally localized wannier orbitals and the extended hubbard model for twisted bilayer graphene, Phys. Rev. X 8, 031087 (2018).
[11] J. Liu, J. Liu, and X. Dai, Pseudo landau level representation of twisted bilayer graphene: Band topology and implications on the correlated insulating phase, Physical Review B 99, 155415 (2019).
[12] G. Tarnopolsky, A. J. Kruchkov, and A. Vishwanath, Origin of Magic Angles in Twisted Bilayer Graphene, Physical Review Letters 122, 106405 (2019).
[13] Z.-D. Song and B. A. Bernevig, MATBG as Topological Heavy Fermion: I. Exact Mapping and Correlated
Insulators, arXiv e-prints, arXiv:2111.05865 (2021), arXiv:2111.05865 [cond-mat.str-el].

[14] J. Wang, Y. Zheng, A. J. Millis, and J. Cano, Chiral approximation to twisted bilayer graphene: Exact intravalley inversion symmetry, nodal structure, and implications for higher magic angles, Physical Review Research 3, 1 (2021).

[15] K. Kim, A. DaSilva, S. Huang, B. Fallahazad, S. Largentis, T. Taniguchi, K. Watanabe, B. J. LeRoy, A. H. MacDonald, and E. Tutuc, Tunable moiré bands and strong correlations in small-twist-angle bilayer graphene, Proceedings of the National Academy of Sciences of the United States of America 114, 3364 (2017).

[16] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, Unconventional superconductivity in magic-angle graphene superlattices, Nature 556, 43 (2018).

[17] Y. Cao, V. Fatemi, A. Demir, S. Fang, S. L. Tomarken, J. Y. Luo, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, E. Kaxiras, R. C. Ashoori, and P. Jarillo-Herrero, Correlated insulator behaviour at half-filling in magic-angle graphene superlattices, Nature 556, 80 (2018).

[18] X. Lu, P. Stepanov, W. Yang, M. Xie, M. A. Aamir, I. Das, C. Urgell, K. Watanabe, T. Taniguchi, G. Zhang, A. Bachtold, A. H. MacDonald, and D. K. Efetov, Superconductors, orbital magnets and correlated states in magic-angle bilayer graphene, Nature 574, 653 (2019), 1903.06513.

[19] M. Yankowitz, S. Chen, H. Polshyn, Y. Zhang, K. Watanabe, T. Taniguchi, D. Graf, A. F. Young, and C. R. Dean, Tuning superconductivity in twisted bilayer graphene, Science 363, 1059 (2019), 1808.07865.

[20] Y. Xie, B. Lian, B. Jäck, X. Liu, C. L. Chiu, K. Watanabe, T. Taniguchi, B. A. Be nevig, and A. Yazdani, Spectroscopic signatures of many-body correlations in magic-angle bilayer graphene, Nature 572, 101 (2019), 1906.09274.

[21] Y. Choi, J. Kemmer, Y. Peng, A. Thomson, H. Arora, R. Polski, Y. Zhang, H. Ren, J. Alicea, G. Refael, F. von Oppen, K. Watanabe, T. Taniguchi, and S. Nadji Perge, Electronic correlations in twisted bilayer graphene near the magic angle, Nature Physics 15, 1174 (2019), 1901.02997.

[22] Y. Jiang, X. Lai, K. Watanabe, T. Taniguchi, K. Haule, J. Mao, and E. Y. Andrei, Charge order and broken rotational symmetry in magic-angle twisted bilayer graphene, Nature 573, 91 (2019), 1904.10153.

[23] A. Kerelsky, L. J. McGilly, D. M. Kennes, L. Xian, M. Yankowitz, S. Chen, K. Watanabe, T. Taniguchi, J. Hone, C. Dean, A. Rubio, and A. N. Pasupathy, Maximized electron interactions at the magic angle in twisted bilayer graphene, Nature 572, 95 (2019).

[24] A. L. Sharpe, E. J. Fox, A. W. Barnard, J. Finney, K. Watanabe, T. Taniguchi, M. A. Kastner, and D. Goldhaber-Gordon, Emergent ferromagnetism near three-quarters filling in twisted bilayer graphene, Science 365, 605 (2019), 1901.03520.

[25] Y. Cao, D. Chowdhury, D. Rodan-Legrain, O. Rubies-Bigorda, K. Watanabe, T. Taniguchi, T. Senthil, and P. Jarillo-Herrero, Strange Metal in Magic-Angle Graphene with near Planckian Dissipation, Physical Review Letters 124, 76801 (2020), 1901.03710.

[26] M. Serlin, C. L. Tschirhart, H. Polshyn, Y. Zhang, J. Zhu, K. Watanabe, T. Taniguchi, L. Balents, and A. F. Young, Intrinsic quantized anomalous Hall effect in a moiré heterostructure, Science 367, 900 (2020), 1907.00261.

[27] D. Wong, K. P. Nuckolls, M. Oh, B. Lian, Y. Xie, S. Jeon, K. Watanabe, T. Taniguchi, B. A. Bernevig, and A. Yazdani, Cascade of electronic transitions in magic-angle twisted bilayer graphene, Nature 582, 198–202 (2020).

[28] K. P. Nuckolls, M. Oh, D. Wong, B. Lian, K. Watanabe, T. Taniguchi, B. A. Bernevig, and A. Yazdani, Strongly correlated chern insulators in magic-angle twisted bilayer graphene, Nature 588, 610 (2020).

[29] Y. Choi, H. Kim, Y. Peng, A. Thomson, C. Lewandowski, R. Polski, Y. Zhang, H. S. Arora, K. Watanabe, T. Taniguchi, et al., Correlation-driven topological phases in magic-angle twisted bilayer graphene, Nature 589, 536 (2021).

[30] Y. Saito, J. Ge, L. Rademaker, K. Watanabe, T. Taniguchi, D. A. Abanin, and A. F. Young, Hofstadter subband ferromagnetism and symmetry-broken chern insulators in twisted bilayer graphene, Nature Physics 17, 478 (2021).

[31] I. Das, X. Lu, J. Herzog-Arbeitman, Z.-D. Song, K. Watanabe, T. Taniguchi, B. A. Bernevig, and D. K. Efetov, Symmetry broken chern insulators and magic series of rashba-like landau level crossings in magic angle bilayer graphene, Nat. Phys. (2021).

[32] S. Wu, Z. Zhang, K. Watanabe, T. Taniguchi, and E. Y. Andrei, Chern insulators, van hove singularities and topological flat bands in magic-angle twisted bilayer graphene, Nature Materials 20, 488 (2021).

[33] M. Oh, K. P. Nuckolls, D. Wong, R. L. Lee, X. Liu, K. Watanabe, T. Taniguchi, and A. Yazdani, Evidence for unconventional superconductivity in twisted bilayer graphene, Nature (London) 600, 240 (2021), arXiv:2109.13944 [cond-mat.supr-con].

[34] M. Ochi, M. Koshino, and K. Kuroki, Possible correlated insulating states in magic-angle twisted bilayer graphene under strongly competing interactions, Phys. Rev. B 98, 081102 (2018).

[35] F. Guinea and N. R. Walet, Electrostatic effects, band distortions, and superconductivity in twisted graphene bilayers, Proceedings of the National Academy of Sciences 115, 13174 (2018).

[36] J. W. F. Venderbos and R. M. Fernandes, Correlations and electronic order in a two-orbital honeycomb lattice model for twisted bilayer graphene, Phys. Rev. B 98, 245103 (2018).

[37] B. Lian, Z. Wang, and B. A. Bernevig, Twisted bilayer graphene: A phonon-driven superconductor, Phys. Rev. Lett. 122, 257002 (2019).

[38] F. Wu, A. H. MacDonald, and I. Martin, Theory of phonon-mediated superconductivity in twisted bilayer graphene, Phys. Rev. Lett. 121, 257001 (2018).

[39] H. Isobe, N. F. Yuan, and L. Fu, Unconventional superconductivity and density waves in twisted bilayer graphene, Physical Review X 8, 041041 (2018).

[40] A. Thomson, S. Chatterjee, S. Sachdev, and M. S. Scheurer, Triangular antiferromagnetism on the honeycomb lattice of twisted bilayer graphene, Physical Review B 98, 10.1103/physrevb.98.075109 (2018).

[41] J. F. Dodaro, S. A. Kivelson, Y. Schattner, X.-Q. Sun, and C. Wang, Phases of a phenomenological model of twisted bilayer graphene, Physical Review B 98, 075154 (2018).
[42] J. Gonzalez and T. Stauber, Kohn-luttinger superconductivity in twisted bilayer graphene, Physical review letters 122, 026801 (2019).

[43] N. F. Yuan and L. Fu, Model for the metal-insulator transition in graphene superlattices and beyond, Physical Review B 98, 045103 (2018).

[44] J. Kang and O. Vafek, Strong Coupling Phases of Partially Filled Twisted Bilayer Graphene Narrow Bands, Physical Review Letters 122, 246401 (2019).

[45] N. Bultinck, E. Khalaf, S. Liu, S. Chatterjee, A. Vishwanath, and M. P. Zaletel, Ground State and Hidden Symmetry of Magic-Angle Graphene at Even Integer Filling, Phys. Rev. X 10, 031034 (2020).

[46] K. Seo, V. N. Kotov, and B. Uchoa, Ferromagnetic mott state in twisted graphene bilayers at the magic angle, Phys. Rev. Lett. 122, 246402 (2019).

[47] K. Hejazi, X. Chen, and L. Balents, Hybrid wannier chern bands in magic angle twisted bilayer graphene and the quantized anomalous hall effect (2021).

[48] E. Khalaf, S. Chatterjee, N. Bultinck, M. P. Zaletel, and A. Vishwanath, Charged skyrmions and topological origin of superconductivity in magic-angle graphene, Science Advances 7, eaab5299 (2021), arXiv:2004.06038 [cond-mat.str-el].

[49] F. Xie, Z. Song, B. Lian, and B. A. Bernevig, Topology-bound superfluid weight in twisted bilayer graphene, Phys. Rev. Lett. 124, 167002 (2020).

[50] A. Julku, T. J. Peltonen, L. Liang, T. T. Heikkilä, and P. Törmä, Superfluid weight and berezinskii-kosterlitz-thouless transition temperature of twisted bilayer graphene, Physical Review B 101, 10.1103/physrevb.101.060505 (2020).

[51] X. Hu, T. Hyart, D. I. Pikulin, and E. Rossi, Geometric and conventional contribution to the superfluid weight in twisted bilayer graphene, Phys. Rev. Lett. 123, 237002 (2019).

[52] J. H. Pixley and E. Y. Andrei, Ferromagnetism in magic-angle graphene, Science 365, 543 (2019), https://science.sciencemag.org/content/365/6453/543.full.pdf.

[53] M. Xie and A. H. MacDonald, Nature of the correlated insulator states in twisted bilayer graphene, Phys. Rev. Lett. 124, 097601 (2020).

[54] Y. Zhang, K. Jiang, Z. Wang, and F. Zhang, Correlated insulating phases of twisted bilayer graphene at commensurate filling fractions: A hartree-fock study, Phys. Rev. B 102, 035136 (2020).

[55] R. M. Fernandes and J. W. F. Venderbos, Nematicity with a twist: Rotational symmetry breaking in a moiré superlattice, Science Advances 6, 10.1126/sciadv.aba8834 (2020), https://advances.sciencemag.org/content/6/32/aba8834.full.pdf.

[56] B. A. Bernevig, Z. D. Song, N. Regnault, and B. Lian, Twisted bilayer graphene. III. Interacting Hamiltonian and exact symmetries, Physical Review B 103, 1 (2021).

[57] B. Lian, Z.-D. Song, N. Regnault, D. K. Efetov, A. Yazdani, and B. A. Bernevig, Twisted bilayer graphene. iv. exact insulator ground states and phase diagram, Physical Review B 103, 10.1103/physrevb.103.205414 (2021).

[58] B. A. Bernevig, B. Lian, A. Coskun, F. Xie, N. Regnault, and Z.-D. Song, Twisted bilayer graphene. v. exact analytic many-body excitations in coulomb Hamiltonians: Charge gap, goldstone modes, and absence of cooper pairing, Physical Review B 103, 10.1103/physrevb.103.205415 (2021).

[59] F. Xie, A. Cowsik, Z.-D. Song, B. Lian, B. A. Bernevig, and N. Regnault, Twisted bilayer graphene. vi. an exact diagonalization study at nonzero integer filling, Physical Review B 103, 10.1103/physrevb.103.205416 (2021).

[60] G. W. Burg, J. Zhu, T. Taniguchi, K. Watanabe, A. H. MacDonald, and E. Tutuc, Correlated Insulating States in Twisted Double Bilayer Graphene, Physical Review Letters 123, 197702 (2019), 1907.10106.

[61] C. Shen, Y. Chu, Q. S. Wu, N. Li, S. Wang, Y. Zhao, J. Tang, J. Liu, J. Tian, K. Watanabe, T. Taniguchi, R. Yang, Z. Y. Meng, D. Shi, O. V. Yazyev, and G. Zhang, Correlated states in twisted double bilayer graphene, Nature Physics 16, 520 (2020).

[62] X. Liu, Z. Hao, E. Khalaf, J. Y. Lee, Y. Ronen, H. Yoo, D. Haei Najafabadi, K. Watanabe, T. Taniguchi, A. Vishwanath, and P. Kim, Tunable spin-polarized correlated states in twisted double bilayer graphene, Nature 583, 221 (2020).

[63] Y. Cao, D. Rodan-Legrain, O. Rubies-Bigorda, J. M. Park, K. Watanabe, T. Taniguchi, and P. Jarillo-Herrero, Tunable correlated states and spin-polarized phases in twisted bilayer–bilayer graphene, Nature 583, 215 (2020).

[64] E. Khalaf, A. J. Kruchkov, G. Tarnopolsky, and A. Vishwanath, Magic angle hierarchy in twisted graphene multilayers, Phys. Rev. B 100, 085109 (2019).

[65] C. Mora, N. Regnault, and B. A. Bernevig, Flatbands and Perfect Metal in Trilayer Moiré Graphene, Phys. Rev. Lett. 123, 026402 (2019).

[66] Z. Hao, A. M. Zimmerman, P. Ledwith, E. Khalaf, D. H. Najafabadi, K. Watanabe, T. Taniguchi, A. Vishwanath, and P. Kim, Electric field–tunable superconductivity in alternating-twist magic-angle trilayer graphene, Science 371, 1133 (2021), https://science.sciencemag.org/content/371/6534/1133.full.pdf.

[67] J. M. Park, Y. Cao, K. Watanabe, T. Taniguchi, and P. Jarillo-Herrero, Tunable strongly coupled superconductivity in magic-angle twisted trilayer graphene, Nature 590, 249 (2021).

[68] Y. Zhang, R. Polski, C. Lewandowski, A. Thomson, Y. Peng, Y. Choi, H. Kim, K. Watanabe, T. Taniguchi, J. Alicea, F. von Oppen, G. Refael, and S. Nadji, Peruge, Ascendence of Superconductivity in Magic-Angle Graphene Multilayers, arXiv e-prints , arXiv:2112.09270 (2021), arXiv:2112.09270 [cond-mat.supr-con].

[69] J. M. Park, Y. Cao, L. Xia, S. Sun, K. Watanabe, T. Taniguchi, and P. Jarillo-Herrero, Magic-Angle Multilayer Graphene: A Robust Family of Moiré Superconductors, arXiv e-prints , arXiv:2112.10760 (2021), arXiv:2112.10760 [cond-mat.supr-con].

[70] G. Chen, A. L. Sharpe, P. Gallagher, I. T. Rosen, E. J. Fox, L. Jiang, B. Lyu, H. Li, K. Watanabe, T. Taniguchi, J. Jung, Z. Shi, D. Goldhaber-Gordon, Y. Zhang, and F. Wang, Signatures of tunable superconductivity in a trilayer graphene moiré superlattice, Nature 572, 215 (2019).

[71] G. Chen, L. Jiang, S. Wu, B. Lyu, H. Li, B. L. Chittari, K. Watanabe, T. Taniguchi, Z. Shi, J. Jung, Y. Zhang, and F. Wang, Evidence of a gate-tunable Mott insulator in a trilayer graphene moiré superlattice, Nature Physics 15, 237 (2019).

[72] G. Chen, A. L. Sharpe, E. J. Fox, Y. H. Zhang, S. Wang, L. Jiang, B. Lyu, H. Li, K. Watanabe, T. Taniguchi, Z. Shi, T. Senthil, D. Goldhaber-Gordon, Y. Zhang, and
F. Wang, Tunable correlated Chern insulator and ferromagnetism in a moiré superlattice, Nature 579, 56 (2020).

[73] H. Zhou, T. Xie, T. Taniguchi, K. Watanabe, and A. F. Young, Superconductivity in rhombohedral trilayer graphene, Nature (London) 598, 434 (2021), arXiv:2106.07640 [cond-mat.mes-hall].

[74] L. Wang, E. M. Shih, A. Ghiotto, L. Xian, D. A. Rhodes, C. Tan, M. Claassen, D. M. Kennes, Y. Bai, B. Kim, K. Watanabe, T. Taniguchi, X. Zhu, J. Hone, A. Rubio, A. N. Pasupathy, and C. R. Dean, Correlated electronic phases in twisted bilayer transition metal dichalcogenides, Nature Materials 19, 861 (2020).

[75] E. C. Regan, D. Wang, C. Jin, M. I. Bakti Utama, B. Gao, X. Wei, S. Zhao, W. Zhao, Z. Zhang, K. Yumigeta, M. Blei, J. D. Carlström, K. Watanabe, T. Taniguchi, S. Tongay, M. Crommie, A. Ruobil, A. N. Pasupathy, and C. R. Dean, Mott and generalized Wigner crystal states in WSe₂/WS₂ moiré superlattices, Nature 579, 359 (2020).

[76] P. Wang, G. Yu, Y. H. Kwan, Y. Jia, S. Klemenz, F. Alexandre Cevallos, R. Singha, T. Devakul, K. Watanabe, T. Taniguchi, S. L. Sondhi, R. J. Cava, L. M. Schoop, S. A. Parameswaran, and S. Wu, One-Dimensional Luttinger Liquids in a Two-Dimensional Moiré Lattice, arXiv e-prints, arXiv:2109.04637 (2021), arXiv:2109.04637 [cond-mat.mes-hall].

[77] P. Moon and M. Koshino, Optical absorption in twisted bilayer graphene, Physical Review B - Condensed Matter and Materials Physics 87, 1 (2013).

[78] N. N. Nam and M. Koshino, Lattice relaxation and energy band modulation in twisted bilayer graphene, Physical Review B 96, 1 (2017), 1706.03908.

[79] S. Carr, S. Fang, Z. Zhu, and E. Kaxiras, Exact continuum model for low-energy electronic states of twisted bilayer graphene, Physical Review Research 1, 1 (2019), 1901.03420.

[80] A. Bernevig, Z. D. Song, N. Regnault, and B. Lian, Twisted bilayer graphene. I. Matrix elements, approximations, perturbation theory, and a K·p two-band model, Physical Review B 103, 10.1103/PhysRevB.103.205411 (2021).

[81] J. Sichau, M. Prada, T. Anlauf, T. J. Lyon, B. Bosnjak, L. Tiemann, and R. H. Blick, Resonance Microwave Measurements of an Intrinsic Spin-Orbit Coupling Gap in Graphene: A Possible Indication of a Topological State, Physical Review Letters 122, 46403 (2019).

[82] J. C. Slater and G. F. Koster, Simplified lcao method for the periodic potential problem, Phys. Rev. 94, 1498 (1954).

[83] E. McCann and V. I. Fal’ko, Landau-level degeneracy and quantum hall effect in a graphite bilayer, Phys. Rev. Lett. 96, 086805 (2006).

[84] Z.-D. Song, B. Lian, N. Regnault, and B. A. Bernevig, Twisted bilayer graphene. ii. stable symmetry anomaly, Phys. Rev. B 103, 205412 (2021).

[85] E. Tang, J.-W. Mei, and X.-G. Wen, High-temperature fractional quantum hall states, Phys. Rev. Lett. 106, 236802 (2011).

[86] G. Xu, B. Lian, and S.-C. Zhang, Intrinsic quantum anomalous hall effect in the kagome lattice $\mathbb{C}_2\mathbb{Z}_3\mathbb{Z}_2$, Phys. Rev. Lett. 115, 186802 (2015).

[87] H. C. Po, H. Watanabe, and A. Vishwanath, Fragile Topology and Wannier Obstructions, Physical Review Letters 121, 126402 (2018).

[88] J. Cano, B. Bradlyn, Z. Wang, L. Elcoro, M. G. Vergniory, C. Felser, M. I. Aroyo, and B. A. Bernevig, Topology of disconnected elementary band representations, Phys. Rev. Lett. 120, 266401 (2018).

[89] A. Bouhon, A. M. Black-Schaffer, and R.-J. Slager, Wilson loop approach to fragile topology of split elementary band representations and topological crystalline insulators with time-reversal symmetry, Phys. Rev. B 100, 195135 (2019).

[90] Y. Yu, X. L. Qi, A. Bernevig, Z. Fang, and X. Dai, Equivalent expression of $\mathbb{C}_2\mathbb{Z}_3\mathbb{Z}_2$ topological invariant for band insulators using the non-Abelian Berry connection, Phys. Rev. B 84, 075119 (2011).

[91] A. Alexandradinata, X. Dai, and B. A. Bernevig, Wilson-loop characterization of inversion-symmetric topological insulators, Phys. Rev. B 89, 155114 (2014).

[92] G. W. Semenoff, Condensed-Matter simulation of a three-Dimensional anomaly, Physical Review Letters 53, 2449 (1984).

[93] A. H. Castro Neto, F. Guinea, N. M. Peres, K. S. Novoselov, and A. K. Geim, The electronic properties of graphene, Reviews of Modern Physics 81, 109 (2009), 0709.1163.

[94] S. Bravyi, D. P. DiVincenzo, and D. Loss, Schrieffer-Wolff transformation for quantum many-body systems, Annals of Physics 326, 2793 (2011), 1105.0675.
Appendices

A. Microscopic Hamiltonian matrix elements

In this appendix, we derive Eqs. (6) and (9) for the intra- and inter-layer microscopic Hamiltonian matrix elements. Recall that $L$ is the Bravais lattice of monolayer graphene, $P$ is its reciprocal lattice, BZ is the Brillouin zone, $L_l = R_{-i	heta/2} L$, and $P_l = R_{-i	heta/2} P$. The Bloch states $|k,l,\alpha\rangle$ are defined by Eq. (3) and satisfy the normalization condition Eq. (4). We first derive Eq. (6) under the simplifying assumption $\mu = 0$ so that Eq. (5) becomes $\langle r', l, \alpha'| H | r, l, \alpha \rangle = t_+ (r' + \tau_\alpha' - r - \tau_\alpha)$. Using the identity

$$\frac{1}{|BZ|} \sum_{r \in L} e^{i k \cdot r} = \sum_{G \in P} \delta^2(k - G), \quad (A1)$$

where $|BZ|$ is the area of BZ, we compute

$$\langle k', l, \alpha'| H | k, l, \alpha \rangle = \frac{1}{|BZ|} \sum_{r,r' \in L} e^{-i k' \cdot (r' + \tau_\alpha')} e^{i k \cdot (r + \tau_\alpha)} t_+ (r' + \tau_\alpha' - r - \tau_\alpha)$$

$$= \frac{1}{|BZ|} \sum_{r' \in L} \sum_{r \in L} e^{-i r' \cdot (k' - k)} e^{-i k' \cdot \tau_\alpha'} e^{i k \cdot (r - \tau_\alpha')} t_+ (r + \tau_\alpha' - \tau_\alpha)$$

$$= \sum_{G \in P} \delta^2(k' - k - G_l) \sum_{r \in L} e^{-i k' \cdot \tau_\alpha'} e^{i k \cdot (-r + \tau_\alpha')} t_+ (r + \tau_\alpha' - \tau_\alpha)$$

$$= \sum_{G \in P} \delta^2(k' - k - G_l) e^{-i G_l \cdot \tau_\alpha} \sum_{r \in L} e^{-i k \cdot (r' + \tau_\alpha' - \tau_\alpha)} t_+ (r + \tau_\alpha' - \tau_\alpha)$$

$$= \langle k', l, \alpha'| k, l, \alpha \rangle \sum_{r \in L + \tau_\alpha' - \tau_\alpha} e^{-i (R_{i\theta/2} k) \cdot r} t_+ (r), \quad (A2)$$

Note that we have used the rotational symmetry of the $t_+$ function in the last step. When $\mu \neq 0$, the Hamiltonian is modified by subtraction of $\mu$ times the identity. As a result, the general form of the matrix element is

$$\langle k', l, \alpha'| H | k, l, \alpha \rangle = \langle k', l, \alpha'| k, l, \alpha \rangle \left( -\mu + \sum_{r \in L + \tau_\alpha' - \tau_\alpha} e^{-i (R_{i\theta/2} k) \cdot r} t_+ (r) \right) \quad (A3)$$

which is Eq. (6).

Next, we derive Eq. (9). Using Eq. (A1) and the identities

$$t_-(r) = \int \frac{d^2 q}{(2\pi)^2} \hat{t}_-(q) e^{i q \cdot r} \quad (A4)$$

$$|\Omega| |BZ| = (2\pi)^2,$$

where $|\Omega|$ is the area of the primitive unit cell $\Omega$ of $L$, we compute

$$\langle k', -l, \alpha'| H | k, l, \alpha \rangle = \frac{1}{|BZ|} \sum_{r \in L_{-l}} \sum_{r' \in L_l} e^{-i k' \cdot (r' + \tau_\alpha')} e^{i k \cdot (r + \tau_\alpha)} t_- (r' + \tau_\alpha' - r - \tau_\alpha)$$

$$= \frac{1}{|BZ|} \sum_{r \in L_{-l}} \sum_{r' \in L_l} \int \frac{d^2 q}{(2\pi)^2} \hat{t}_-(q) e^{-i k' \cdot (r' + \tau_\alpha')} e^{i k \cdot (r + \tau_\alpha)} e^{i q \cdot (r' + \tau_\alpha' - r - \tau_\alpha)}$$

$$= |BZ| \int \frac{d^2 q}{(2\pi)^2} \hat{t}_-(q) e^{i \tau_\alpha' \cdot (q - k')} e^{i \tau_\alpha \cdot (k - q)} \sum_{G \in P_{-l}} \delta^2(q - k' - G_{-l}) \sum_{G \in P_l} \delta^2(k - q + G_l) \quad (A5)$$

$$= \sum_{G_{-l} \in P_{-l}} \sum_{G \in P_l} \frac{\hat{t}_-(k + G_l)}{|\Omega|} e^{i \tau_\alpha' \cdot G_{-l}} e^{-i \tau_\alpha \cdot G} e^{i \tau_\alpha' \cdot G} \delta^2(k + G_l - k' - G_{-l})$$

which is Eq. (9).
B. Dirac cones

In this appendix, we derive Eq. (7). Since this equation is an approximation of Eq. (6) and both equations depend on the crystal momentum \( k \) only through \( R_{\theta/2} k \), it suffices to consider the case \( \theta = 0 \). That is, we need to show that the single particle Hamiltonian for monolayer graphene at \( \mathbf{K} + \mathbf{p} \) takes the form

\[
h v_F \sigma_0 \cdot \mathbf{p} + O(|\mathbf{p}|^2)
\]

(B1)

when the chemical potential is chosen appropriately. Although this is well known, the most common derivation employs a model of graphene that has only first or second order hopping (for example, see Refs. [92, 93]). We will now give an argument based on symmetry to show that Eq. (B1) holds with arbitrary order hopping. This is similar to the symmetry argument given in Sec. III in the case of twisted bilayer graphene near commensuration.

For monolayer graphene, we consider an orthonormal basis of spinless \( p_z \) orbitals \( |\mathbf{r}, \alpha \rangle \) for \( \mathbf{r} \in L \) and \( \alpha \in \{A, B\} \) localized at \( \mathbf{r} + \tau_\alpha \). We ignore the electron spin because of the weak spin-orbit coupling in graphene [81]. The Bloch states are defined by

\[
|\mathbf{k}, \alpha \rangle = \frac{1}{\sqrt{|BZ|}} \sum_{\mathbf{r} \in L} e^{ik (\mathbf{r} + \tau_\alpha)} |\mathbf{r}, \alpha \rangle
\]

(B2)

for crystal momentum vectors \( \mathbf{k} \), and satisfy the normalization condition

\[
\langle \mathbf{k}', \alpha' | \mathbf{r}, \alpha \rangle = \delta_{\alpha', \alpha} \sum_{\mathbf{G} \in P} \delta^2 (\mathbf{k}' - \mathbf{k} - \mathbf{G}) e^{-i \mathbf{r} \cdot \mathbf{G}}.
\]

(B3)

We consider a microscopic Hamiltonian \( H_{\text{mono}} \) with matrix elements

\[
\langle \mathbf{r}', \alpha' | H_{\text{mono}} | \mathbf{r}, \alpha \rangle = t_+ (\mathbf{r}' + \tau_\alpha - \mathbf{r} - \tau_\alpha) - \mu \delta_{\mathbf{r}', \mathbf{r}} \delta_{\alpha', \alpha}
\]

(B4)

the where \( \mu \) is a chemical potential and \( t_+ : \mathbb{R}^2 \rightarrow \mathbb{R} \) is a rotationally symmetric function (i.e. \( t_+ (\mathbf{r}) \) depends only on \( |\mathbf{r}| \)). The symmetries of \( H_{\text{mono}} \) are generated by the unitary operators \( C_{6z} \) (rotation by \( \pi/3 \) about \( \hat{z} \)), \( M_y \) (reflection across the \( xz \) plane), and the anti-unitary operator \( T \) (time-reversal). These operators take the form

\[
C_{6z} |\mathbf{k}, \alpha \rangle = |R_{\pi/3} \mathbf{k}, -\alpha \rangle
\]

\[
M_y |\mathbf{k}, \alpha \rangle = |R^* \mathbf{k}, -\alpha \rangle
\]

\[
T |\mathbf{k}, \alpha \rangle = |-\mathbf{k}, \alpha \rangle
\]

(B5)

where \( R^x \) denotes reflection across the \( x \) axis. The symmetry subgroup that preserves the high-symmetry crystal momentum \( \mathbf{K} \) is generated by \( C_{2z} T, C_{3z} \), and \( M_y \), where \( C_{2z} = C_{6z} \) and \( C_{3z} = C_{6z}^2 \). Using Eq. (B3) we find

\[
C_{2z} T |\mathbf{K} + \mathbf{p}, \alpha \rangle = |\mathbf{K} + \mathbf{p}, -\alpha \rangle
\]

(B6)

\[
C_{3z} |\mathbf{K} + \mathbf{p}, \alpha \rangle = e^{i(2\pi/3)\alpha} |\mathbf{K} + R_{2\pi/3} \mathbf{p}, \alpha \rangle
\]

(B7)

\[
M_y |\mathbf{K} + \mathbf{p}, \alpha \rangle = |\mathbf{K} + R^* \mathbf{p}, -\alpha \rangle.
\]

(B8)

If we expand the matrix elements of \( H_{\text{mono}} \) to second order around \( \mathbf{K} \), we find

\[
\langle \mathbf{K} + \mathbf{p}', \alpha' | H_{\text{mono}} | \mathbf{K} + \mathbf{p}, \alpha \rangle = \langle H_{\text{mono}}(\mathbf{p}) \rangle_{\alpha', \alpha} + O(|\mathbf{p}|^2) \delta^2 (\mathbf{p}' - \mathbf{p})
\]

(B9)

where \( H_{\text{mono}}(\mathbf{p}) \) is a Hermitian \( 2 \times 2 \) matrix that is linear in \( \mathbf{p} \). Requiring

\[
[C_{2z} T, H_{\text{mono}}] = [C_{3z}, H_{\text{mono}}] = [M_y, H_{\text{mono}}] = 0
\]

(B10)

implies

\[
H_{\text{mono}}(\mathbf{p}) = \sigma_x \overline{H_{\text{mono}}(\mathbf{p})} \sigma_x
\]

(B11)

\[
e^{-i(2\pi/3)\sigma_z} H_{\text{mono}}(R_{2\pi/3} \mathbf{p}) e^{i(2\pi/3)\sigma_z}
\]

(B12)

\[
= \sigma_x H_{\text{mono}}(R^* \mathbf{p}) \sigma_x
\]

(B13)
where we use the notation $\overline{M}$ for the complex conjugate of a matrix $M$. We now expand $\mathcal{H}_{\text{mono}}$ in Pauli matrices as

$$
\begin{align*}
\mathcal{H}_{\text{mono}}(p) &= \hbar^0_0 \sigma_0 + \hbar^x_0 \sigma_x + \hbar^y_0 \sigma_y + \hbar^z_0 \sigma_z \\
&+ (\hbar^0_x \sigma_0 + \hbar^x_x \sigma_x + \hbar^y_x \sigma_y + \hbar^z_x \sigma_z) p_x \\
&+ (\hbar^0_y \sigma_0 + \hbar^x_y \sigma_x + \hbar^y_y \sigma_y + \hbar^z_y \sigma_z) p_y
\end{align*}
$$

(B14)

where the $h$ coefficients are real. First, we choose the value of $\mu$ so that $\hbar^0_0 = 0$. Next, Eq. (B11) implies $\hbar^0_x = \hbar^x_x = \hbar^z_x = 0$ and Eq. (B12) implies $\hbar^0_y = \hbar^x_y = \hbar^y_y = 0$ and $\hbar^y_y + i \hbar^y_y = i(\hbar^x_x + i \hbar^y_y)$. If we define $v_F$ and $\phi_F$ by $h v_F e^{i \phi_F} = \hbar^x_x + i \hbar^y_y$ we have

$$
\mathcal{H}_{\text{mono}}(p) = hv_F \sigma_{\phi_F} \cdot p.
$$

(B15)

Finally, Eq. (B13) implies $\phi_F = 0$ so the Hamiltonian is described by Eq. (B1). We conclude that the $C_{2z} T$ and $C_{3z}$ symmetries imply that $\mathcal{H}_{\text{mono}}$ takes the form of a Dirac cone and $M_y$ symmetry determines the rotation angle of the Dirac cone.

**C. Equivalent configurations**

Note that the microscopic Hamiltonian in Eq. (5) is uniquely determined up to unitary equivalence by the relative positions of the carbon atoms in the $xy$ plane and their partitioning into two layers. We will therefore consider systems differing only by an isometry of the $xy$ plane and a relabeling of the basis states to be equivalent. This leads to significant redundancy in the specification of bilayer configurations, as we will now show.

With angle and translation parameters $(\theta, d)$, the atoms are located at sites

$$
\{R_{\theta/2}(r + \tau_\alpha) - d/2 | r \in L, \alpha \in \{A, B\} \} \cup \{R_{\theta/2}(r + \tau_\alpha) + d/2 | r \in L, \alpha \in \{A, B\} \}
$$

(C1)

where the two terms indicate the top and bottom layers. Since this set and partitioning is invariant under the mapping $\theta \mapsto -\theta$, $d \mapsto -d$ (with an interchange of the two layers) the configurations with parameters $(\theta, d)$ and $(-\theta, -d)$ are equivalent.

Next, consider the configuration with parameters $(\theta + \pi/3, R_{-\pi/6} d)$. If we rotate the whole system by the angle $\pi/6$, the bottom layer atoms are located at

$$
\{R_{\theta/2 + \pi/3}(r + \tau_\alpha) + d/2 | r \in L, \alpha \in \{A, B\} \}
$$

(C2)

and the top layer atoms are located at

$$
\{R_{-\theta/2}(r + \tau_\alpha) - d/2 | r \in L, \alpha \in \{A, B\} \}.
$$

(C3)

Since $R_{\pi/3} L = L$ and $R_{\pi/3} \tau_\alpha - \tau_{-\alpha} \in L$, the bottom layer atoms are equivalently located at

$$
\{R_{\theta/2}(r + \tau_\alpha) + d/2 | r \in L, \alpha \in \{A, B\} \}.
$$

(C4)

Since these locations now match Eq. (C1), we see that the configurations with parameters $(\theta, d)$ and $(\theta + \pi/3, R_{-\pi/6} d)$ are equivalent. As a result of these equivalences, we can restrict $\theta$ to the interval $[0, \pi/3)$ and note that the configurations $(\theta, d)$ and $(\pi/3 - \theta, -R_{-\pi/6} d)$ are equivalent.

Next, consider the configuration with parameters $(\theta, d + X)$ for a vector $X \in \mathbb{R}^2$. If we translate the whole system by $X/2$, the atoms are located at sites

$$
\{R_{-\theta/2}(r + \tau_\alpha) - d/2 | r \in L, \alpha \in \{A, B\} \} \cup \{R_{\theta/2}(r + \tau_\alpha) + d/2 + X | r \in L, \alpha \in \{A, B\} \}.
$$

(C5)

If $X \in L_-$ then this matches Eq. (C1) so the configurations with parameters $(\theta, d)$ and $(\theta, d + X)$ are equivalent. Similarly, if we translate the whole system by $-X/2$, we see that when $X \in L_+$ the configurations with parameters $(\theta, d)$ and $(\theta, d + X)$ are equivalent. Putting these results together, we see that whenever $X \in L_- + L_+$, the configurations with parameters $(\theta, d)$ and $(\theta, d + X)$ are equivalent.

We show in App. D 2 that when $\theta$ is a commensurate angle, $L_- + L_+$ is a Bravais lattice whose reciprocal lattice is $P_{\perp} \cap P_{\parallel}$. Furthermore, it follows from the results of App. D 6 that for commensurate $\theta$, no set $S$ larger than $L_- + L_+$ has the property that the configurations with parameters $(\theta, d)$ and $(\theta, d + X)$ are equivalent for all $d \in \mathbb{R}^2$ and all $X \in S$. On the other hand, we show in App. E that when $\theta$ is not a commensurate angle, $L_- + L_+$ is a dense subset of $\mathbb{R}^2$. Since the Hamiltonian depends continuously on $\theta$, it follows that for incommensurate $\theta$ the configurations with parameters $(\theta, 0)$ and $(\theta, d)$ are equivalent for all $d \in \mathbb{R}^2$. 


D. Properties of commensurate configurations

Using a combination of elementary number theory and symmetry arguments, these appendices enumerate and characterize the commensurate configurations of TBG. The approach taken in Apps. D 1 and D 2 is similar to that in Ref. [2], but we include detailed derivations for completeness. We follow the notations of Secs. II A and II B.

1. Enumeration of commensurate configurations

We first seek to enumerate the commensurate configurations. Recall that \( a_1, a_2 \) are primitive vectors for \( L \) and \( b_1, b_2 \) are primitive vectors for \( P \), as illustrated in Fig. 1. Let \( a \) and \( b \) denote matrices with columns \((a_1, a_2)\) and \((b_1, b_2)\) respectively. Explicitly, we have

\[
a = a_0 \begin{pmatrix} \sqrt{3} & \sqrt{3}/2 \\ 0 & -3/2 \end{pmatrix}, \quad b = \frac{2\pi}{a_0} \begin{pmatrix} \sqrt{3}/3 & 0 \\ 1/3 & -2/3 \end{pmatrix}.
\]

(D1)

Recall from Sec. II B that the bilayer system is commensurate when \( L_- \cap L_+ \neq \{0\} \), and in this case \( L_- \cap L_+ \) is the commensuration superlattice. \( L_\cdash \cap L_\plus \neq \{0\} \) is equivalent to the existence of nonzero integer vectors \( u_\plus \) and \( u_- \) such that

\[
u_\plus = a^{-1} R_\theta a u_-.
\]

(D2)

Similarly, \( P_- \cap P_\plus \neq \{0\} \) is equivalent to the existence of nonzero integer vectors \( v_\plus \) and \( v_- \) such that

\[
v_\plus = b^{-1} R_\theta b v_-.
\]

(D3)

Note that

\[
a^{-1} R_\theta a = \begin{pmatrix} x_0 + y_0 & 2 y_0 \\ -2 y_0 & x_0 - y_0 \end{pmatrix}, \quad b^{-1} R_\theta b = \begin{pmatrix} x_0 - y_0 & 2 y_0 \\ -2 y_0 & x_0 + y_0 \end{pmatrix}
\]

(D4)

where \( x_0 = \cos \theta, y_0 = \frac{1}{\sqrt{3}} \sin \theta \). It follows that the bilayer system is commensurate if and only if \( x_0 \) and \( y_0 \) are both rational, which is equivalent to the \( L_- \cap L_+ \neq \{0\} \) and \( P_- \cap P_\plus \neq \{0\} \).

From here on, we will use \( \theta_0 \) in place of \( \theta \) when we assume the system is commensurate in order to match the notation of Sec. II B. If the system is commensurate, then \((x_0, y_0)\) is a rational point on the ellipse \( x^2 + 3 y^2 = 1 \). Unless \((x_0, y_0) = (1, 0)\), the line through \((x_0, y_0)\) and \((1, 0)\) intersects the \( y \) axis at a rational point \((0, m/n)\) where \( m, n \) are relatively prime integers with \( n > 0 \). Solving \( x^2 + 3 y^2 = 1 \) simultaneously with \( x = -\frac{2}{m} y + 1 \) yields

\[
x_0 = \frac{3 m^2 - n^2}{3 m^2 + n^2}, \quad y_0 = \frac{2 mn}{3 m^2 + n^2}.
\]

(D6)

The special case \((x_0, y_0) = (1, 0)\) corresponds to \((m, n) = (1, 0)\). By the results of App. C, we can restrict \( \theta_0 \in [0, \pi/3) \) so that \( m > n \geq 0 \) and \( \theta_0 = \cos^{-1}(x_0) \).
2. Commensuration lattices

We now determine the primitive vectors and reciprocal lattices of \( L_- \cap L_+ \) and \( P_- \cap P_+ \) assuming \( \theta_0 \) is a commensurate angle. We have

\[
a^{-1}R_{\theta_0}a = \frac{1}{N} \begin{pmatrix} \alpha & \beta \\ -\beta & \gamma \end{pmatrix} \tag{D7}
\]

\[
b^{-1}R_{\theta_0}b = \frac{1}{N} \begin{pmatrix} \gamma & \beta \\ -\beta & \alpha \end{pmatrix} \tag{D8}
\]

\[
\alpha = (m+n)(3m-n)/d_0 \tag{D9}
\]

\[
\beta = 4mn/d_0 = \alpha - \gamma \tag{D10}
\]

\[
\gamma = (m-n)(3m+n)/d_0 \tag{D11}
\]

\[
N = (3m^2 + n^2)/d_0 \tag{D12}
\]

where \( d_0 \) is the greatest common divisor of the numerators of \( \alpha, \beta, \gamma, N \). Note that \( \alpha \) should not be confused with the model parameter defined in Eq. (64) and used in the main text. If \( 3 \nmid n \) (i.e. 3 does not divide \( n \)) then the numerator of \( N \) is 1 (mod 3) so \( 3 \nmid d_0 \). On the other hand, if \( 3 \mid n \) then \( 3 \nmid d_0 \) but 9 \nmid \( d_0 \) since \( 3 \nmid m \). In either case \( 3 \nmid N \). If one of \( m \) and \( n \) is even, then the numerator of \( N \) is odd so \( d_0 \) is odd. On the other hand, if \( m \) and \( n \) are both odd then \( 4 \nmid d_0 \), but considering the numerator of \( \beta \) we see that \( 8 \nmid d_0 \). If \( p \) is a prime divisor of \( d_0 \) other than 2 then considering the numerator of \( \beta \), we see that \( p \mid m \) or \( p \mid n \) but not both. Considering the numerator of \( N \), we see that \( p = 3 \). We conclude

\[
d_0 = \gcd(4mn, 3m^2 + n^2) = \begin{cases} 1 & \text{if } (2\nmid n \text{ or } 2\mid m) \text{ and } 3 \nmid n \\ 3 & \text{if } (2\nmid n \text{ or } 2\mid m) \text{ and } 3\mid n \\ 4 & \text{if } 2 \nmid n \text{ and } 2 \nmid m \text{ and } 3 \nmid n \\ 12 & \text{if } 2 \nmid n \text{ and } 2 \nmid m \text{ and } 3 \nmid n \end{cases} \tag{D13}
\]

so that \( \gcd(\beta, N) = 1 \). Also, since \( \det(a^{-1}R_{\theta_0}a) = 1 \) we have \( \alpha \gamma + \beta^2 = N^2 \).

Assume for now that \( (m, n) \neq (1, 0) \) so that \( \beta \neq 0 \). Writing \( u_- \) in components as \( u_- = x\hat{x} + y\hat{y} \) for integers \( x, y \), Eq. (D2) becomes

\[
\frac{1}{N} \begin{pmatrix} \alpha & \beta \\ -\beta & \gamma \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \in \mathbb{Z}^2 \tag{D14}
\]

which is in turn equivalent to the pair of congruences

\[
\alpha x + \beta y \equiv 0 \pmod{N} \tag{D15}
\]

\[
-\beta x + \gamma y \equiv 0 \pmod{N}. \tag{D16}
\]

Since \( \beta \neq 0 \) and \( \gcd(\beta, N) = 1 \), we can multiply Eq. (D16) through by \( \beta \). However since \( -\beta^2 \equiv \alpha \gamma \pmod{N} \), we see that this equation is implied Eq. (D15). Furthermore, Eq. (D15) can be solved as

\[
x = n_1 \tag{D17}
\]

\[
y = n_1(-\beta^{-1} \alpha) + n_2 N \tag{D18}
\]

for integers \( n_1, n_2 \), where \( \beta^{-1} \) is the smallest non-negative integer such that \( \beta^{-1}\beta = 1 \pmod{N^2} \). As a result, the set of integer vectors \( u \) such that \( a^{-1}R_{\theta_0}au \) is an integer vector forms a Bravais lattice with primitive vectors

\[
u_1 = \hat{x} - \beta^{-1} \alpha \hat{y} \tag{D19}
\]

\[
u_2 = N\hat{y}. \tag{D20}
\]

In the case \( (m, n) = (1, 0) \), \( a^{-1}R_{\theta_0}a = I \), \( N = 1 \), and \( \beta^{-1} = 0 \) so this result still holds. The image of this lattice under \( a^{-1}R_{\theta_0}a \) is also a Bravais lattice with corresponding primitive vectors

\[
u_1^+ = a^{-1}R_{\theta_0}a\nu_1^- = -\alpha \rho \hat{x} + (\beta \rho - \beta^{-1} N)\hat{y} \tag{D21}
\]

\[
u_2^+ = a^{-1}R_{\theta_0}a\nu_2^- = \beta \hat{x} + \gamma \hat{y} \tag{D22}
\]

\[
\rho = (\beta^{-1}\beta - 1)/N \in \mathbb{N}Z. \tag{D23}
\]
We conclude that the commensuration superlattice takes the form
\[ L_+ \cap L_- = \{ R_{-\theta_0/2} a(n_1 u_1^1 + n_2 u_2^1) | n_1, n_2 \in \mathbb{Z} \} = \{ R_{\theta_0/2} a(n_1 u_1^1 + n_2 u_2^1) | n_1, n_2 \in \mathbb{Z} \}. \] (D24)

Note that the unit cell of \( L_+ \cap L_- \) has area \( N|\Omega| \).

We can use this result to compute the reciprocal lattice of \( L_+ \cap L_- \). Let this reciprocal lattice be called \( \tilde{P} \) and note that primitive vectors for \( \tilde{P} \) can be given by
\[ \tilde{u}_1 = \frac{1}{N} R_{-\theta_0/2} b(\gamma \hat{x} - \beta \hat{y}) = R_{\theta_0/2} b \hat{x} \] (D25)
\[ \tilde{u}_2 = R_{-\theta_0/2} b(-\beta \rho/N + \beta^{-1}) \hat{x} - (\alpha \rho/N) \hat{y} = \frac{1}{N} R_{\theta_0/2} b(-\beta^{-1} \alpha \hat{x} + \hat{y}). \] (D26)

Since \( \rho/N \) is an integer, \( \tilde{u}_1 \in P_- \), \( \tilde{u}_2 \in P_+ \) so \( \tilde{P} \subset P_- + P_+ \). However, by the definition of the reciprocal lattice \( P_- + P_+ \subset \tilde{P} \) so that \( \tilde{P} = P_- + P_+ \). Note that the unit cell for \( \tilde{P} \) has area \( |BZ|/N \).

Since Eqs. (D7) and (D8) are related by the interchange of \( \alpha \) and \( \gamma \), corresponding results for the reciprocal lattices can be obtained by interchanging \( \alpha \) and \( \gamma \). The set of integer vectors \( v \) such that \( b^{-1} R_{\theta_0} b v \) is an integer vector forms a Bravais lattice with primitive vectors
\[ v_1^- = \hat{x} - \beta^{-1} \gamma \hat{y} \] (D27)
\[ v_2^- = N \hat{y} \] (D28)
and the image of this lattice under \( b^{-1} R_{\theta_0} b \) is also a Bravais lattice with corresponding primitive vectors
\[ v_1^+ = b^{-1} R_{\theta_0} b v_1^- = -\gamma \rho \hat{x} + (\beta \rho - \beta^{-1} N) \hat{y} \] (D29)
\[ v_2^+ = b^{-1} R_{\theta_0} b v_2^- = \beta \hat{y} + \alpha \hat{x}. \] (D30)

We conclude
\[ P_+ \cap P_- = \{ R_{-\theta_0/2} b(n_1 v_1^1 + n_2 v_2^1) | n_1, n_2 \in \mathbb{Z} \} = \{ R_{\theta_0/2} b(n_1 v_1^- + n_2 v_2^-) | n_1, n_2 \in \mathbb{Z} \}, \] (D31)
the reciprocal lattice of \( P_- \cap P_+ \) is \( L_- + L_+ \), and the unit cell of \( P_- \cap P_+ \) has area \( N|BZ| \).

3. Equivalences between top and bottom \( K \) and \( K' \) points

We will now derive Eqs. (12) to (14) starting with Eq. (14). By Eq. (2),
\[ K_j = R_{-\theta_0/2} K \]
\[ = R_{-\theta_0/2}(2b_1 + b_2)/3 \] (D32)
\[ = R_{-\theta_0/2} b(2 \hat{x} + \hat{y})/3 \]
and similarly \( K'_j = R_{-\theta_0/2} b(\hat{x} + 2 \hat{y}) \), so that \( K_j - K'_j = R_{-\theta_0/2} (\hat{x} - \hat{y})/3 \). Examining the primitive vectors \( \tilde{u}_1 \) and \( \tilde{u}_2 \) for \( P_- + P_+ \) in Eqs. (D25) and (D26), we see that if \( R_{-\theta_0/2} b v \in P_- + P_+ \), where \( v \) is a rational vector then the denominators of \( v \cdot \hat{x} \) and \( v \cdot \hat{y} \) must divide \( N \). Since \( 3 \not| N \), it follows that \( K_j - K'_j \not\in P_- + P_+ \), which is Eq. (14).

Next, since \( 3 \not| N \) there is an integer \( k \in \{0, 1, 2\} \) such that
\[ kN = 2 + \beta^{-1} \gamma \pmod{3} \] (D33)
so that by Eqs. (D27) and (D28) we have
\[ v_1^- + k v_2^- = \hat{x} + 2 \hat{y} \pmod{3}. \] (D34)
Recalling that \( v_j^+ = b^{-1} R_{\theta_0} b v_j^- \) for \( j = 1, 2 \) we then have
\[ K_- = -R_{\theta_0/2} b(v_1^- + k v_2^-)/3 + G_- \] (D35)
\[ = -R_{-\theta_0/2} b(v_1^+ + k v_2^+)/3 + G_- \] (D36)
\[ K'_- = R_{\theta_0/2} b(v_1^- + k v_2^-)/3 + G'_- \] (D37)
\[ = R_{-\theta_0/2} b(v_1^+ + k v_2^+)/3 + G'_-. \] (D38)
for some \( \mathbf{G}_-, \mathbf{G}'_- \in \mathcal{P}_- \). Multiplying these equations by \( R_{-\theta_0} \), we find

\[
\mathbf{K} = -R_{-\theta_0/2}b(v^+ - k\mathbf{v}^-)/3 + \mathbf{G}_+ \tag{D39}
\]

\[
\mathbf{K}' = R_{-\theta_0/2}b(v^+ - k\mathbf{v}^-)/3 + \mathbf{G}'_+ \tag{D40}
\]

where \( \mathbf{G}_+ = R_{-\theta_0}\mathbf{G}_- \in \mathcal{P}_+ \) and \( \mathbf{G}'_+ = R_{-\theta_0}\mathbf{G}'_- \in \mathcal{P}_+ \). Note that

\[
\mathbf{K} - \mathbf{K}_- = R_{-\theta_0/2}b(v^+ - v^- + k(\mathbf{v}^- - \mathbf{v}^+))/3 + \mathbf{G}_+ - \mathbf{G}_- \tag{D41}
\]

so \( \mathbf{K} - \mathbf{K}_- \in \mathcal{P}_+ + \mathcal{P}_+ \) if and only if \( R_{-\theta_0/2}b(v^+ - v^- + k(\mathbf{v}^- - \mathbf{v}^+))/3 \in \mathcal{P}_+ + \mathcal{P}_+ \). By the same argument as before, we see that \( \mathbf{K} - \mathbf{K}_- \in \mathcal{P}_+ + \mathcal{P}_+ \) if and only if

\[
v^+ + kv^+ = \hat{x} + 2\hat{y} \pmod{3} \tag{D42}
\]

in which case we also have \( \mathbf{K}' - \mathbf{K}'_- \in \mathcal{P}_+ + \mathcal{P}_+ \). Similarly, \( \mathbf{K} + \mathbf{K}_- \in \mathcal{P}_+ + \mathcal{P}_+ \) if and only if

\[
v^+ + kv^+ = 2\hat{x} + \hat{y} \pmod{3} \tag{D43}
\]

in which case we also have \( \mathbf{K}' + \mathbf{K}'_- \in \mathcal{P}_+ + \mathcal{P}_+ \).

Using Eqs. (D29), (D30) and (D33), \( \alpha\gamma + \beta^2 = N^2 = 1 \pmod{3} \), and \( \beta = \alpha - \gamma \), one can show

\[
v^+ + kv^+ = N(\alpha + \gamma)(2\hat{x} + \hat{y}) \pmod{3} \tag{D44}
\]

Additionally, using Eq. (D13) we find

\[
N(\alpha + \gamma) = 2(9m^4 - n^4)/d_0^2 \tag{D45}
\]

\[
= \begin{cases} 
1 & \text{if } 3 \nmid n \\
2 & \text{if } 3|n.
\end{cases}
\]

Let \( (\mathbf{J}_-, \mathbf{J}_-') \) denote \( (\mathbf{K}_-, \mathbf{K}_-') \) when \( 3|n \) and \( (\mathbf{K}'_-, \mathbf{K}_-) \) when \( 3 \nmid n \). We then conclude \( \mathbf{K} + \mathbf{J}_-, \mathbf{K}' + \mathbf{J}'_- \in \mathcal{P}_+ + \mathcal{P}_+ \), which is equivalent to Eqs. (12) and (13).

4. Pairs of complementary commensurate configurations

It follows from App. C that when \( \theta_0 \) is a commensurate angle, \( \pi/3 - \theta_0 \) is also a commensurate angle. We will now prove this statement another way and consider an important relationship between the two configurations that is used in Sec. II.B.

Returning to the notation of App. D1, let

\[
x_1 = \cos(\pi/3 - \theta_0) = \frac{1}{2}(x_0 + 3y_0) \tag{D46}
\]

\[
y_1 = \frac{1}{\sqrt{3}} \sin(\pi/3 - \theta_0) = \frac{1}{2}(x_0 - y_0). \tag{D47}
\]

Since \( \theta_0 \) is a commensurate angle, \( x_0 \) and \( y_0 \) are rational, and therefore \( x_1 \) and \( y_1 \) are rational. It follows that \( \pi/3 - \theta_0 \) is also commensurate. If \( (x_0, y_0) \) corresponds to the integer pair \( (m_0, n_0) \) and \( (x_1, y_1) \) corresponds to the integer pair \( (m_1, n_1) \) then

\[
\frac{m_1}{n_1} = \frac{y_1}{1 - x_1} = \frac{3m_0^2 - 2m_0n_0 - n_0^2}{3(m_0 - n_0)^2}. \tag{D48}
\]

If \( 3|n_0 \) then \( 3 \nmid m_0 \) so the denominator of this fraction is divisible by 3 exactly once. However, the numerator is also divisible by 3 so we conclude \( 3 \nmid n_1 \). On the other hand, suppose \( 3 \nmid n_0 \). It is straightforward to see that the largest power of 3 dividing the numerator is the same as the largest power of 3 dividing \( m_0 - n_0 \), so we conclude \( 3|n_1 \). As a result, in one of the commensurate configurations corresponding to \( \theta_0 \) and \( \pi/3 - \theta_0 \) we have \( (\mathbf{J}_-, \mathbf{J}_-) = (\mathbf{K}_-, \mathbf{K}_-) \), and in the other we have \( (\mathbf{J}_-, \mathbf{J}_-) = (\mathbf{K}'_-, \mathbf{K}_-) \).
5. The lattices $Q_+$ and $Q_0$

In this section, we prove Eq. (32), find the minimal norm elements of $(\mathbf{K}_- + P_-) \cap (\mathbf{K}_+ + P_+)$, and derive the forms of $L_- \cap L_+ \cap P_-$, $L_- + L_+$, and $P_- + P_+$. As explained in Sec. II B, we assume $3|n$ so that $\mathbf{J}_- = \mathbf{K}_-$. Since $(\mathbf{K}_- + P_-) \cap (\mathbf{K}_+ + P_+)$ is closed under addition by elements of $P_- \cap P_+$ and has the property that the difference of any two elements is in $P_- \cap P_+$, we must have

$$(\mathbf{K}_- + P_-) \cap (\mathbf{K}_+ + P_+) = \mathbf{k}_0 + P_- \cap P_+$$

(D49)

for some vector $\mathbf{k}_0$. Since $P_- \cap P_+$ is a triangular lattice, $\mathbf{k}_0 + P_- \cap P_+$ has at most three elements of minimal norm. However, since $(\mathbf{K}_- + P_-) \cap (\mathbf{K}_+ + P_+)$ has 3-fold rotational symmetry and does not contain 0, it must have exactly three elements of minimal norm. Since $(\mathbf{K}_- + P_-) \cap (\mathbf{K}_+ + P_+)$ additionally has symmetry under reflection across the vector $\mathbf{K}$, one of the elements of minimal norm must be proportional to $\mathbf{K}$. Since the unit cell of $P_- \cap P_+$ has area $N|\text{BZ}|$, we conclude $P_- \cap P_+ = \sqrt{N}\mathbf{P}$ and the element of minimal norm proportional to $\mathbf{K}$ must be $\mathbf{Q}_1 = s\sqrt{N}\mathbf{K}$ where $s$ is 1 or $-1$. The other two elements of minimal norm are $\mathbf{Q}_2 = R_{2\pi/3}\mathbf{Q}_1$ and $\mathbf{Q}_3 = R_{4\pi/3}\mathbf{Q}_1$, and we can write

$$(\mathbf{K}_- + P_-) \cap (\mathbf{K}_+ + P_+) = s\sqrt{N}\mathbf{K} + P_- \cap P_+.$$  

(D50)

Recalling from App. D 2 that the reciprocal lattice of $P_- \cap P_+$ is $L_- + L_+$, it follows that $L_- + L_+ = L/\sqrt{N}$. Applying the same argument to the real space lattices, we see that $L_- \cap L_+ = \sqrt{N}\mathbf{L}$ so that $P_- + P_+ = P/\sqrt{N}$.

We will now determine the sign $s$. We have $s\sqrt{N}\mathbf{K} - \mathbf{K}_i \in P_1$ or equivalently $(s\sqrt{N}R_{i\theta_0/2} - I)\mathbf{K} \in P$. Using the half-angle formulas and the results of Apps. D 1 and D 2 we find

$$\cos(\theta_0/2) = \frac{m\sqrt{3}}{\sqrt{d_0N}},$$

(D51)

$$\sin(\theta_0/2) = \frac{n}{\sqrt{d_0N}}$$

(D52)

$$(s\sqrt{N}R_{i\theta_0/2} - I)\mathbf{K} = \frac{4\pi\sqrt{3}}{9a_0} \left((sm\sqrt{3}/d_0 - 1)\hat{x} + (snl/\sqrt{d_0})\hat{y}\right).$$

(D53)

For comparison,

$$n_1\mathbf{b}_1 + n_2\mathbf{b}_2 = \frac{4\pi\sqrt{3}}{9a_0} \left((3n_1/2)\hat{x} + (n_1/2 - n_2)\sqrt{3}\hat{y}\right).$$

(D54)

By Eq. (D13), when $m \pm n$ is odd, we have $d_0 = 3$ so the equation $(s\sqrt{N}R_{i\theta_0/2} - I)\mathbf{K} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2$ has a solution if and only if $sm = 1 \mod 3$. When $m \pm n$ is even, we have $d_0 = 12$ so the same equation now has a solution if and only if $sm = 2 \mod 3$. We summarize both cases by saying

$s = \frac{m \pm n}{\sqrt{d_0/3}} \mod 3$ and $s = \pm 1.$

(D55)

6. AA, AB, BA stacking commensurate configurations

We say that a commensurate configuration has AA stacking if there is an A sublattice atom on the top layer that is directly above some A sublattice atom on the bottom layer. Similarly we say that a commensurate configuration has AB (BA) stacking if there is a B (A) sublattice atom on the top layer that is directly above some A (B) sublattice atom on the bottom layer. For the commensurate configuration with $\theta_0 = 0$, it is clear that $\mathbf{d} = 0$ (i.e. no inter-layer translation) corresponds to AA stacking, $\mathbf{d} = a_0\hat{y}$ corresponds to AB stacking, and $\mathbf{d} = -a_0\hat{y}$ corresponds to BA stacking. We will now derive a generalization of this correspondence for commensurate configurations with $3|n$.

We first consider AA stacking. In this case, there is a pair of vectors $\mathbf{r}_+ \in L_+$ and $\mathbf{r}_- \in L_-$ such that $\mathbf{r}_+ + \tau_A^+ = \mathbf{r}_- + \tau_A^+$.
r_- + \tau_A^- \in L_- + L_+. Using Eq. (D52), we have
\begin{align*}
\tau_A^+ - \tau_A^- &= (R_{-\theta_0/2} \tau_A - d/2) - (R_{\theta_0/2} \tau_A + d/2) \\
&= -(R_{\theta_0/2} - R_{-\theta_0/2})(a_0 \hat{y}) - d \\
&= 2 \sin(\theta_0/2)(a_0 \hat{x}) - d \\
&= \frac{2n}{\sqrt{d_0 N}} a_0 \hat{x} - d \\
&= n'a_1/\sqrt{N} - d
\end{align*}

(D56)

where \(n' = 2n/\sqrt{3L_0}\) is an integer since \(3|n\) and \(d_0 \in \{3, 12\}\) by Eq. (D13). Since we found in App. D5 that \(L_- + L_+ = L/\sqrt{N}\) we see that \(\tau_A^+ - \tau_A^- \in L_- + L_+\) if and only if \(d \in L_- + L_+\). We conclude that AA stacking corresponds to \(d \in L_- + L_+\). Since \(\tau_B = R_{-\pi/3} \tau_A\) and \(a_2 = R_{-\pi/3} a_1\) we have
\begin{align*}
\tau_B^- - \tau_B^+ &= n'a_2/\sqrt{N} - d
\end{align*}

(D57)

so that \(\tau_B^+ - \tau_B^- \in L_- + L_+\) if and only if \(d \in L_- + L_+\). It follows that AA stacking can equivalently be defined by saying that there is a B sublattice atom on the top layer that is directly above some B sublattice atom on the bottom layer. A commensurate configuration with AA stacking is shown in Fig. 2.

Next, we consider AB and BA stacking. In AB stacking, there are vectors \(r_l \in L_l\) such that \(r_+ + \tau_B^+ = r_- + \tau_B^-\), or equivalently \(\tau_B^+ - \tau_B^- \in L_- + L_+\). Similarly, BA stacking is equivalent to \(\tau_A^+ - \tau_B^- \in L_- + L_+\). Using Eqs. (D51) and (D52), we have
\begin{align*}
\tau_A^+ - \tau_B^- &= -(R_{\theta_0/2} \tau_B - R_{-\theta_0/2} \tau_A) - ld \\
&= -(R_{-\pi/6}(R_{(\theta_0 - \pi/3)/2} - R_{-(\theta_0 - \pi/3)/2}) \tau_A) - ld \\
&= 2 \sin((l\theta_0 - \pi/3)/2) R_{-\pi/6}(a_0 \hat{x}) - ld \\
&= (l \sin(\theta_0/2) \sqrt{3} - \cos(\theta_0/2))(\tau_B - \tau_A) - ld \\
&= -m'(\tau_B - \tau_A)/\sqrt{N} - ld
\end{align*}

(D58)

where \(m' = (m - ln)/\sqrt{d_0/3}\) is an integer with \(m' = s\) (mod 3) by Eq. (D55). It follows that \(\tau_A^+ - \tau_B^- \in L_- + L_+\) if and only if \(d \in \frac{m'a_0 \hat{y}}{\sqrt{N}} + L_- + L_+\) so that AB stacking corresponds to \(d \in \frac{m'a_0 \hat{y}}{\sqrt{N}} + L_- + L_+\) and BA stacking corresponds to \(d \in -\frac{m'a_0 \hat{y}}{\sqrt{N}} + L_- + L_+\). Commensurate configurations with AB and BA stacking are shown in Fig. 11.
E. \( L_- + L_+ \) and \( P_- + P_+ \) are dense for incommensurate \( \theta \)

Suppose \( \theta \) is an incommensurate angle. Recall from App. D 1 that this implies \( x_0 \) and \( y_0 \) are not both rational. It follows from Eq. (D4) that both columns and both rows of the matrix \( a^{-1}R_\theta a \) contain an irrational value. It is well known that for any irrational number \( z \), the set of fractional parts of integer multiples of \( z \) is dense in the interval \([0, 1)\). Equivalently, the set of integer linear combinations of 1 and \( z \) is dense in \( \mathbb{R} \). It follows that the set of integer linear combinations of \( a^{-1}R_\theta a x, a^{-1}R_\theta a y \), \( x \), \( y \) is dense in \( \mathbb{R}^2 \). Since the linear map \( R_{-\theta/2}a \) is continuous and density is preserved under continuous maps, we conclude that \( L_- + L_+ \) is dense in \( \mathbb{R}^2 \). A similar argument using Eq. (D5) shows that \( P_- + P_+ \) is dense in \( \mathbb{R}^2 \) as well.

F. Properties of the distance function \( d \)

1. We consider item 1 in Sec. II C which claims \( d(k, l, k, l) = 0 \). If we write \( k + G_l = (k + G_{-l} \) where \( G_l = G_{-l} = 0 \), we then have \( d(k, l, k, l) = |G_{-l}| = 0 \).

2. We consider item 2 in Sec. II C which claims \( d(k, l, k', l') = d(k', l', k, l) \). If \( k' - k \notin P_- + P_+ \) then \( d(k, l, k', l') = \infty = d(k', l', k, l) \). Otherwise, suppose \( k + G_l = k' + G_{-l} \) for some \( G_- \in P_- \), \( G_+ \in P_+ \). There are two cases to consider:

   - If \( l' = -l \) then \( k' + G_{l'} = k + G_{-l} \) so that
     \[
     d(k, l, k', l') = |k + G_l| = |k' + G_{l'}| = d(k', l', k, l). \quad \text{(F1)}
     \]
   - If \( l' = l \) then \( k' - G_{l'} = k - G_{-l} \) so that
     \[
     d(k, l, k', l') = |G_{-l}| = |-G_{-l}| = d(k', l', k, l). \quad \text{(F2)}
     \]

3. We consider item 3 in Sec. II C which claims

   \[
   d(k, l, k'', l'') \leq d(k, l, k', l') + d(k', l', k'', l''). \quad \text{(F3)}
   \]

When either term on the right hand side is \( \infty \), the inequality is trivially satisfied. If the left hand side is \( \infty \) then \( k'' - k \notin P_- + P_+ \). This implies that at least one of the terms on the right hand side must be \( \infty \) as well, so the inequality is satisfied.

Otherwise, suppose

\[
\begin{align*}
  k + G_l &= k' + G_{-l} \quad \text{(F4)}
  k' + G_{l'} &= k'' + G_{-l'} \quad \text{(F5)}
\end{align*}
\]

for some \( G_- \land G'_+ \in P_- \) and \( G_+, G'_+ \in P_+ \). It follows that

\[
  k + G_l + G_{l'} = k'' + G_{-l} + G_{-l'} \quad \text{(F6)}
\]

We now consider three cases:

(a) Suppose \( l = l' = l'' \) and without loss of generality we take \( l = l' = l'' = + \). Then \( d(k, l, k', l') = |G_-| \), \( d(k', l', k'', l'') = |G_+| \), \( k + G_l'' = k'' + G_{-l}'' \) where

\[
\begin{align*}
  G_{l''} &= G_- + G'_- \quad \text{(F7)}
  G_{l''} &= G_+ + G'_+. \quad \text{(F8)}
\end{align*}
\]

We then have

\[
\begin{align*}
  d(k, l, k'', l'') &= |G_{l''}| \\
  &= |G_- + G'_-| \\
  &\leq d(k, l, k', l') + d(k', l', k'', l''). \quad \text{(F9)}
\end{align*}
\]
(b) Suppose \( l = l' \neq l'' \) and without loss of generality we take \( l = l' = +, l'' = - \). Then \( d(k, l, k', l') = |G_-| \), \( d(k', l', k'', l'') = |k'' + G'_-| \) and \( k + G''_+ = k'' + G''_{l} \) where

\[
G''_+ = G_- + G'_-
\]

\[
G''_- = G_+ + G'_+
\]

We then have

\[
d(k, l, k', l') = |k'' + G''_+| = |G_- + (k'' + G'_-)| \leq d(k, l, k', l') + d(k', l', k'', l'').
\]

(c) Suppose \( l = l' \neq l'' \) and without loss of generality we take \( l = l'' = +, l' = - \). Then \( d(k, l, k', l') = |k' + G_-| \), \( d(k', l', k'', l'') = |k' + G'_-| \) and \( k + G''_l = k' + G''_{l'} \) where

\[
G''_l = G_- - G'_-
\]

\[
G''_{l'} = G_+ - G'_+
\]

We then have

\[
d(k, l, k', l'') = |G''_l| = |G_- - G'_-| = |(k' + G_-) - (k' + G'_-)| \leq d(k, l, k', l') + d(k', l', k'', l'').
\]

The last case in which \( l \neq l' = l'' \) follows from the symmetry of \( d \) and the case \( l = l' \neq l'' \).

G. Level sets of \( d \)

In this section we prove the characterization of \( d \) described in Sec. II.D. Recall that \( P_{l}^0 = R_{-\theta_0/2}P \) and that \( \theta = \theta_0 + \delta \theta \) is an incommensurate angle, where \( \theta_0 \) is a commensurate angle and \( \delta \theta \) is small. Let \( k \in \mathbb{R}^2 \), \( l \in \{+, -\} \), and let \( k_0 = R_{\delta \theta/2}k \). Suppose that \( k', l' \) satisfy \( d(k, l, k', l') < \infty \) so that we can write \( k + G_l = k' + G_{-l} \) for unique vectors \( G_\pm \in P_\pm \), \( G_\pm \in P_+ \). Define \( G^0_\pm = R_{-\delta \theta/2}G_\pm \in P_0^0 \) and \( k_0' = k_0 + G^0_l = k_0 + P_0^0 + G^0_{l'} \). We then have

\[
k' - R_{-\delta \theta/2}k_0' = (k + G_l - G_-) - R_{-\delta \theta/2}(k_0 + G^0_l - G^0_-)
\]

\[
= R_{-\delta \theta/2}(k_0 + G^0_l) - R_{-\delta \theta/2}(k_0 + G^0_-)
\]

\[
= -lD(\delta \theta)Q_{-l}
\]

where \( D(\delta \theta) \) is defined by Eq. (19) and

\[
Q_{-l} = k_0 + G^0_- = k_0' + G^0_{-l} \in (k_0 + P_0^0) \cap (k_0' + P_0^0) = Q(k_0, l, k_0', -l).
\]

Similarly,

\[
k' - R_{-\delta \theta/2}k_0' = (k + G_l - G_-) - R_{-\delta \theta/2}(k_0 + G^0_l - G^0_-)
\]

\[
= R_{-\delta \theta/2}G^0_l - R_{-\delta \theta/2}G^0_{-l}
\]

\[
= -lD(\delta \theta)Q_0
\]

where

\[
Q_0 = G^0_{-l} = k_0 - k'_0 + G^0_{l} \in P_0^0 \cap (k_0 - k'_0 + P_0^0) = Q(k_0, l, k'_0, l).
\]

It follows that

\[
k' = R_{-\delta \theta/2}k_0' - lD(\delta \theta)Q_{l'}
\]

where \( Q_{l'} \in Q(k_0, l, k'_0, l') \). Furthermore, the vectors \( k_0' \) and \( Q_{l'} \) are uniquely determined because the vectors \( G_- \) and \( G_+ \) are uniquely determined. Additionally, since \( |Q_{-l}| = |k_0 + G^0_-| = |k + G_l| \) and \( |Q_0| = |G^0_{-l}| = |G_l| \) we have \( d(k, l, k', l') = |Q_{l'}| \). The converse statement can be proved simply by tracing the above argument backwards.
H. Equivalence of small rotations and spatially varying translations

We now derive Eq. (47) which relates the $T$ potential in commensurate and incommensurate configurations. In this section, we denote continuum states $|p, l, \alpha \rangle_c$ and $|r, l, \alpha \rangle_c$ with twist angle $\theta = \theta_0 + \delta \theta$ and translation vector $d$ by $|p, l, \alpha, \delta \theta, d \rangle_c$ and $|r, l, \alpha, \delta \theta, d \rangle_c$, respectively. Since $|p, l, \alpha, 0, d \rangle_c$ is a state with crystal momentum $K_l + p$ which has been shifted by $-ld/2$ we must have

$$
|p, l, \alpha, 0, d \rangle_c = e^{-i(K_l + p) \cdot d/2} |p, l, \alpha, 0 \rangle_c .
$$

Similarly, since $|p, l, \alpha, \delta \theta, 0 \rangle_c$ is a momentum state that has been rotated by $-l \delta \theta/2$, we must have

$$
|p, l, \alpha, \delta \theta, 0 \rangle_c = |R_{l \delta \theta/2} p, l, \alpha, 0 \rangle_c .
$$

By Eq. (40), we then have

$$
|r, l, \alpha, 0, d \rangle = e^{-iK_l \cdot d/2} |r + ld/2, l, \alpha, 0 \rangle
$$

$$
|r, l, \alpha, \delta \theta, 0 \rangle = |R_{l \delta \theta/2} r, l, \alpha, 0 \rangle
$$

so that Eq. (45) implies

$$
|r, l, \alpha, \delta \theta, 0 \rangle = e^{iK_l \cdot D(\delta \theta) r/2} |r, l, \alpha, 0, D(\delta \theta) r \rangle + O(\delta \theta^2).
$$

Next, let the continuum Hamiltonian $\tilde{H}$ with twist angle $\theta = \theta_0 + \delta \theta$ and translation vector $d$ be denoted $\tilde{H}(\delta \theta, d)$. Since the pattern of atoms near position $r$ with $\theta = \theta_0 + \delta \theta$ and $d = 0$ is the same to first order in $\delta \theta$ as the pattern with $\theta = \theta_0$ and $d = D(\delta \theta) r$, we must have

$$
|\langle r' \rangle, \alpha', \delta \theta, 0 \rangle_c \tilde{H}(\delta \theta, 0) |r, l, \alpha, \delta \theta, 0 \rangle_c = \langle r' \rangle, \alpha', 0, D(\delta \theta) r \rangle \tilde{H}(0, D(\delta \theta) r) |r, l, \alpha, 0, D(\delta \theta) r \rangle_c + O(\delta \theta^2)
$$

It follows that

$$
T(r, \delta \theta, 0) = \langle r', +, A, \delta \theta, 0 \rangle_c \langle r, +, B, \delta \theta, 0 \rangle_c \tilde{H}(\delta \theta, 0) \left( \begin{array}{c} \langle r, -, A, \delta \theta, 0 \rangle_c \\ \langle r, -, B, \delta \theta, 0 \rangle_c \end{array} \right)
$$

$$
= e^{-i(K_+ - K_+ \cdot D(\delta \theta) r/2)} \left( \begin{array}{c} \langle r, +, A, 0, D(\delta \theta) r \rangle_c \\ \langle r, +, B, 0, D(\delta \theta) r \rangle_c \end{array} \right) \tilde{H}(0, D(\delta \theta) r) \left( \begin{array}{c} \langle r, -, A, 0, D(\delta \theta) r \rangle_c \\ \langle r, -, B, 0, D(\delta \theta) r \rangle_c \end{array} \right)
$$

$$
+ O(\delta \theta^2)
$$

$$
= e^{i \cos(\theta/2) K_+ \cdot D(\delta \theta) r} T(r, 0, D(\delta \theta) r) + O(\delta \theta^2)
$$

which is equivalent to Eq. (47).

I. Symmetry representations

In this section, we give the representations of the unitary and anti-unitary symmetries of twisted bilayer graphene referred to in Sec. III. For $\theta \neq 0$, the spinless symmetries of the full Hamiltonian are generated by the unitary operators $C_{6z}$ (rotation by $\pi/3$ about $\hat{z}$), $C_{2x}$ (rotation by $\pi$ about $\hat{x}$), and the anti-unitary operator $T$ (time-reversal). These operators take the form

$$
C_{6z} |k, l, \alpha \rangle = |R_{\pi/3} k, l, -\alpha \rangle
$$

$$
C_{2x} |k, l, \alpha \rangle = - |R^x k, l, -\alpha \rangle
$$

$$
T |k, l, \alpha \rangle = - |k, l, \alpha \rangle
$$

where $R^x$ denotes reflection across the $x$ axis. The minus sign for $C_{2x}$ reflects the fact that $|r, l, \alpha \rangle$ are $p_z$ orbitals. The symmetry subgroup preserving valley is generated by $C_{2z} T$, $C_{3z}$, and $C_{2x}$, where $C_{2x} = C_{6z}^3$ and $C_{3z} = C_{6z}^2$. Using Eq. (4), we find

$$
C_{2z} T |K_l + p, l, \alpha \rangle = |K_l + p, l, -\alpha \rangle
$$

$$
C_{3z} |k, l, \alpha \rangle = e^{i(2\pi/3)\alpha} |K + R_{2\pi/3} p, l, \alpha \rangle
$$

$$
C_{2x} |k, l, \alpha \rangle = - |K - l + R^x p, l, -\alpha \rangle .
$$
As a result, the appropriate representations on the $|\mathbf{p}, l, \alpha\rangle_c$ space are

\begin{align*}
C_{2z} |\mathbf{p}\rangle_c &= |\mathbf{p}\rangle_c \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix} \\
C_{3z} |\mathbf{p}\rangle_c &= |R_{2\pi/3}\mathbf{p}\rangle_c e^{i(2\pi/3)\sigma_z} \\
C_{2x} |\mathbf{p}\rangle_c &= |R_x\mathbf{p}\rangle_c \begin{pmatrix} 0 & -\sigma_x \\ -\sigma_x & 0 \end{pmatrix}
\end{align*}

where $|\mathbf{p}\rangle_c$ is defined in Eq. (29).

In the case $\theta = 0$ there is an additional valley preserving unitary symmetry $M_y$ (reflection across the $xz$ plane). This operator has representations

\begin{align*}
M_y |\mathbf{k}, l, \alpha\rangle &= |R_x\mathbf{k}, l, -\alpha\rangle \\
M_y |\mathbf{K} + \mathbf{p}, l, \alpha\rangle &= |\mathbf{K} + R_x\mathbf{p}, l, -\alpha\rangle \\
M_y |\mathbf{p}\rangle_c &= |R_x\mathbf{p}\rangle_c \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix}
\end{align*}

For $\theta$ near 0, $M_y$ can be considered an approximate symmetry.

\section*{J. Determining the model parameters when $\delta \theta = 0$}

Recall from Sec. II E that in the commensurate case, the continuum Hamiltonian approximates the four bands of $H$ nearest the Fermi level at charge neutrality. Explicitly, this model takes the form of a $\mathbf{p}$ dependent $4 \times 4$ matrix as shown in Eq. (58). In order to determine the parameters for this model, we will now describe a method to determine an effective Hamiltonian for these four bands directly from the microscopic Hamiltonian $H$.

Recall from Sec. II B that for commensurate configurations, $H$ is block diagonal with blocks of dimension $4N$. Let $H(\mathbf{p})$ be the Hamiltonian block containing Bloch states $|\mathbf{K}_l + \mathbf{p}, l, \alpha\rangle$ for $l \in \{+,-\}$, $\alpha \in \{A,B\}$. In practice, the $4N \times 4N$ matrix representation for $H(\mathbf{p})$ can be computed accurately from Eqs. (6) and (9) with finitely many terms for each sum as long as the hopping functions $t_+ (\mathbf{r})$ and $t_- (\mathbf{k})$ decay rapidly enough. We diagonalize $H(\mathbf{p})$ as

\begin{align*}
H(\mathbf{p}) &= \sum_{j=1}^{4N} E_j(\mathbf{p}) |\mathbf{p}, j\rangle \langle \mathbf{p}, j|
\end{align*}

for real eigenvalues $E_1(\mathbf{p}) \leq E_2(\mathbf{p}) \leq \cdots \leq E_{4N}(\mathbf{p})$ and orthonormal eigenvectors $|\mathbf{p}, j\rangle$. The indices $j$ from $2N - 1$ to $2N + 2$ correspond to the four bands described by the continuum Hamiltonian.

Define the projection operators

\begin{align*}
P_0(\mathbf{p}) &= \sum_{l=\pm} \sum_{\alpha = \pm} |\mathbf{K}_l + \mathbf{p}, l, \alpha\rangle \langle \mathbf{K}_l + \mathbf{p}, l, \alpha| \\
P_1(\mathbf{p}) &= \sum_{j=2N-1}^{2N+2} |\mathbf{p}, j\rangle \langle \mathbf{p}, j|
\end{align*}

Since the states $|\mathbf{p}, j\rangle$ are almost completely supported on the states $|\mathbf{K}_l + \mathbf{p}, l, \alpha\rangle$, the operators $P_0(\mathbf{p})$ and $P_1(\mathbf{p})$ are nearly the same. It follows that there is a canonical unitary operator $U(\mathbf{p})$ called the direct rotation that satisfies

\begin{align*}
U(\mathbf{p})P_1(\mathbf{p})U^\dagger(\mathbf{p}) &= P_0(\mathbf{p})
\end{align*}

and minimizes the Frobenius norm of $U(\mathbf{p}) - I$ over all unitary operators satisfying Eq. (J3) [94]. The only condition upon which this theorem is dependent is $||P_0(\mathbf{p}) - P_1(\mathbf{p})||_{op} < 1$, which is satisfied in practice. Here, we use the notation $||M||_{op}$ to denote the operator norm of $M$. The direct rotation is given explicitly by

\begin{align*}
U(\mathbf{p}) &= \sqrt{(I - 2P_0(\mathbf{p}))(I - 2P_1(\mathbf{p}))}
\end{align*}
using the hopping functions $t$ are larger but still bounded by $10^{-3.5}$ for $p = 0$. The relative errors for $(m, n) = (1, 0)$ are larger but still bounded by $10^{-1}$ for all $|p|$ values considered, and the relative error at $p = 0$ is less than 0.03. We conclude that $\tilde{H}$ is an accurate model for the four bands of $H$ nearest the Fermi level at charge neutrality for all $d$ and small $p$. Fig. 13 compares the eigenvalues of $H_{\text{eff}}(p)$ and $H_0(p)$ for each commensurate configuration in Tab. II as a function of $p$ for three values of $d$. 

FIG. 12. The maximal relative error between $H_{\text{eff}}(p)$ and $H_0(p)$ as a function of $|p|/|p_0|$ where $\hbar v_F|p_0| = 3|w_0|$ (see Eq. (J7)). The maximum is taken over $d$ in a $10 \times 10$ discretization of a unit cell of $2L/\sqrt{N}$ and five values of $p$ with a given norm.
FIG. 13. Commensurate band structures. The lines use the model in Eqs. (58) and (59) with parameters in Tab. II whereas the dots use the microscopic Hamiltonian in Eqs. (6) and (9). The vector $\mathbf{p}$ ranges linearly from $-3a_0/2$ to $3a_0/2$ where $\hbar v_F p_0 = 3|w_0|\hat{x}$. Recall that $d = 0$ and $d = s\sqrt{N}a_0\hat{y}$ correspond to $AA$ and $AB$ stacking, respectively.
Following Ref. [77], we take

\[ t_+(r) = A_0 e^{(a_0 - |r|)/\delta_0} \]

\[ t_-(r) = A_0 e^{(a_0 - \sqrt{|r|^2 + r_z^2})/\delta_0} \frac{|r|^2}{|r|^2 + r_z^2} + B_0 e^{(r_z - \sqrt{|r|^2 + r_z^2})/\delta_0} \frac{r_z^2}{|r|^2 + r_z^2} \]

where \( A_0 = -2.7 \text{ eV} \) and \( B_0 = 0.48 \text{ eV} \) are transfer integrals, \( r_z = 2.36 a_0 \) is the inter-layer spacing, and \( \delta_0 = 0.318 a_0 \) is chosen so that \( t_+(a_1) \approx t_+(\tau_B - \tau_A)/10 \). Using Eqs. (6) and (7) we find

\[ \hbar v_F / a_0 \approx 3.684 \times 10^3 \text{ eV.} \]

### L. Signs of the parameters and discrete symmetries

We now consider the continuum Hamiltonian \( \hat{H} \) in Eq. (68) as a function \( \hat{H}(\phi_0, w_0, w_1, w_2, \delta \theta, s) \) of the shown parameters. By Eq. (36), we have

\[ \hat{H}(\phi_0, w_0, w_1, w_2, -\delta \theta, s) = \hat{H}(\phi_0, w_0, w_1, w_2, \delta \theta, -s) = -\hat{H}(\phi_0, -w_0, -w_1, -w_2, \delta \theta, s). \]

Similarly, by Eq. (70), we have

\[ \hat{H}(\phi_0 + \pi, w_0, w_1, w_2, \delta \theta, s) = \hat{H}(\phi_0, -w_0, w_1, 2\delta \theta, s). \]

Next, we consider the particle hole operator \( P \), first chiral operator \( C \) (which is often simply called the “chiral operator” [12] when there is no ambiguity), and second chiral operator \( C' \) defined in Ref. [56]

\[ P|p\rangle_c' = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} |p\rangle_c' \]

\[ C|p\rangle_c' = |p\rangle_c' \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} \]

\[ C'|p\rangle_c' = |p\rangle_c' \begin{pmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix} \].

These operators act within the \( K \) valley and the origin of quasi-momentum \( p \) is the \( \Gamma_M \) point of the moiré Brillouin zone. These operators are unitary and satisfy

\[ \hat{P} \hat{H}(\phi_0, w_0, w_1, w_2, \delta \theta, s) \hat{P}^{-1} = -\hat{H}(\phi_0, w_0, w_1, -w_2, \delta \theta, s) \]

\[ \hat{C} \hat{H}(\phi_0, w_0, w_1, w_2, \delta \theta, s) \hat{C}^{-1} = -\hat{H}(\phi_0, -w_0, -w_1, -w_2, \delta \theta, s) \]

\[ \hat{C}' \hat{H}(\phi_0, w_0, w_1, w_2, \delta \theta, s) \hat{C}'^{-1} = -\hat{H}(\phi_0, w_0, -w_1, -w_2, \delta \theta, s). \]

It follows that \( \hat{H} \) is always equivalent up to a sign and a unitary change of basis from the case in which \( s = 1, 0 \leq \phi_0 \leq \pi/2, \) and \( w_0, w_1, w_2, \delta \theta \geq 0, \) so it is sufficient to restrict the parameters in these ranges in calculations.

In particular, we have

\[ C\hat{P} \hat{H}(\phi_0, w_0, w_1, w_2, \delta \theta, s)(CP)^{-1} = \hat{H}(\pi - \phi_0, w_0, w_1, w_2, \delta \theta, s) \].

Therefore, when \( \phi_0 = \pi/2, \) the system has a combined \( CP \) symmetry, although neither \( C \) nor \( P \) is a symmetry. Moreover, noting that the \( CP \) operator map momentum \( p \) to \( -p, \) \( CP \) symmetry implies that the energy spectrum at \( \phi_0 = \pi/2 \) is symmetric between \( p \) and \( -p, \) as can be seen in Fig. 9(d)-(f).
M. Tripod model approximation for magic angle conditions

In this section, we use Eq. (68) to approximate the condition under which the bands of the continuum Hamiltonian nearest the Fermi level at charge neutrality become flat near the \( K_M \) point in the moiré Brillouin zone. Recall from Eqs. (34) and (37) that a continuum state \( |p, \alpha_c \rangle \) has moiré quasi-momentum \( p + lq \) and that \( K_M = q1 \). In order to make the model analytically tractable, we project the Hamiltonian in Eq. (68) into the subspace spanned by the eight states to make the model analytically tractable, we project the Hamiltonian in Eq. (68) into the subspace spanned by the eight states. This projected Hamiltonian is called the “tripod Hamiltonian” \([3, 80]\).

We now consider the case where all these eight states have moiré quasi-momentum equivalent to \( K_M + p \) up to translations by elements of the moiré reciprocal lattice. This projected Hamiltonian is called the “tripod Hamiltonian” \([3, 80]\).

In this section, we use Eq. (68) to approximate the condition under which the bands of the continuum Hamiltonian nearest the Fermi level at charge neutrality become flat near the \( K_M \) point in the moiré Brillouin zone. Recall from Eqs. (34) and (37) that a continuum state \( |p, \alpha_c \rangle \) has moiré quasi-momentum \( p + lq \) and that \( K_M = q1 \). In order to make the model analytically tractable, we project the Hamiltonian in Eq. (68) into the subspace spanned by the eight states to make the model analytically tractable, we project the Hamiltonian in Eq. (68) into the subspace spanned by the eight states. This projected Hamiltonian is called the “tripod Hamiltonian” \([3, 80]\).

We now consider the case where all these eight states have moiré quasi-momentum equivalent to \( K_M + p \) up to translations by elements of the moiré reciprocal lattice. This projected Hamiltonian is called the “tripod Hamiltonian” \([3, 80]\).

In this section, we use Eq. (68) to approximate the condition under which the bands of the continuum Hamiltonian nearest the Fermi level at charge neutrality become flat near the \( K_M \) point in the moiré Brillouin zone. Recall from Eqs. (34) and (37) that a continuum state \( |p, \alpha_c \rangle \) has moiré quasi-momentum \( p + lq \) and that \( K_M = q1 \). In order to make the model analytically tractable, we project the Hamiltonian in Eq. (68) into the subspace spanned by the eight states to make the model analytically tractable, we project the Hamiltonian in Eq. (68) into the subspace spanned by the eight states. This projected Hamiltonian is called the “tripod Hamiltonian” \([3, 80]\).

We now consider the case where all these eight states have moiré quasi-momentum equivalent to \( K_M + p \) up to translations by elements of the moiré reciprocal lattice. This projected Hamiltonian is called the “tripod Hamiltonian” \([3, 80]\).

We now consider the case where all these eight states have moiré quasi-momentum equivalent to \( K_M + p \) up to translations by elements of the moiré reciprocal lattice. This projected Hamiltonian is called the “tripod Hamiltonian” \([3, 80]\).
Using the identities
\[ \sum_{j=1}^{3} \hat{T}_{Q_j}^T \hat{T}_{Q_j} = 3\lambda^2(w_0^2 + w_1^2)I \] \hspace{1cm} (M10)
\[ \sum_{j=1}^{3} \hat{T}_{Q_j}^T (\sigma_0 \cdot q_j') \hat{T}_{Q_j} = 6\lambda^2 w_0 w_1 \sin(\phi_0)I, \]
Eq. (M9) becomes
\[ \left( E' + \frac{E'}{1 - E'^2} 3\lambda^2(w_0^2 + w_1^2) - \frac{1}{1 - E'^2} 6\lambda^2 w_0 w_1 \sin(\phi_0) \right) \psi_0 = 0. \] \hspace{1cm} (M11)

Since \( \psi_0 \neq 0 \), we conclude
\[ E'^3 - E'[1 + 3\lambda^2(w_0^2 + w_1^2)] + 6\lambda^2 w_0 w_1 \sin(\phi_0) = 0. \] \hspace{1cm} (M12)

Note that when \( E' = 1 \), the cubic polynomial in Eq. (M12) takes the value
\[ -3\lambda^2(w_0^2 + w_1^2) + 6\lambda^2 w_0 w_1 \sin(\phi_0) \leq -3\lambda^2(w_0^2 + w_1^2) + 6\lambda^2 |w_0||w_1| = -3\lambda^2(|w_0| - |w_1|)^2 \leq 0 \] \hspace{1cm} (M13)
and when \( E' = -1 \), it takes the value
\[ 3\lambda^2(w_0^2 + w_1^2) + 6\lambda^2 w_0 w_1 \sin(\phi_0) \geq 3\lambda^2(w_0^2 + w_1^2) - 6\lambda^2 |w_0||w_1| = 3\lambda^2(|w_0| - |w_1|)^2 \geq 0. \] \hspace{1cm} (M14)

There is therefore some solution \( E' = E'_0 \) of Eq. (M12) with \( E'_0 \) in the interval \([-1, 1]\). Additionally, when \( |\sin(\phi_0)| < 1 \) or \( |w_0| \neq |w_1| \), we can take \( E'_0 \) in the interval \((-1, 1)\). In this case, we can approximate \( E'^3_0 \approx 0 \) and find
\[ E'_0 \approx \frac{6\lambda^2 w_0 w_1 \sin(\phi_0)}{1 + 3\lambda^2(w_0^2 + w_1^2)} \in (-1, 1). \] \hspace{1cm} (M15)

When \( |\sin(\phi_0)| = 1 \) and \( |w_0| = |w_1| \), it is possible that there is no solution of Eq. (M12) in \((-1, 1)\). We will not consider this case further.

Next, we consider Eq. (M8) with \( p' \neq 0 \). We take \( E' = E'_0 + \delta E' \) and expand to first order in \( \delta E' \) and \( |p'| \). Using \( |p' - q'_j|^2 \approx 1 - 2p' \cdot q'_j \cdot E'^2 \approx E'^2_0 + 2E'_0 \delta E', \) and the fact that \( E'_0 \) solves Eq. (M12), we find
\[ 0 \approx \left( (E'_0 + \delta E')I - \sigma_0 \cdot p' + \sum_{j=1}^{3} \hat{T}_{Q_j}^T \frac{(E'_0 + \delta E')I + \sigma_0 \cdot (p' - q'_j)}{1 - E'^2_0 - 2p' \cdot q'_j - 2E'_0 \delta E'} \hat{T}_{Q_j} \right) \psi_0 \]
\[ = \left( (E'_0 + \delta E')I - \sigma_0 \cdot p' + \sum_{j=1}^{3} \hat{T}_{Q_j}^T \frac{(E'_0 + \delta E')I + \sigma_0 \cdot (p' - q'_j)}{1 - E'^2_0} \hat{T}_{Q_j} \right) \left( 1 + \frac{1}{1 - E'^2_0} \right) \psi_0 \]
\[ \approx ((E'_0 + \delta E')I - \sigma_0 \cdot p')\psi_0 \] \hspace{1cm} (M16)
\[ + \left( \sum_{j=1}^{3} \hat{T}_{Q_j}^T \frac{E'_0 I - \sigma_0 \cdot q'_j \hat{T}_{Q_j}}{1 - E'^2_0} \right) \left( \frac{1}{1 - E'^2_0} \right) \psi_0 \]
\[ \approx \left( \delta E'I - \sigma_0 \cdot p' + \sum_{j=1}^{3} \hat{T}_{Q_j}^T \frac{E'_0 I - \sigma_0 \cdot q'_j \hat{T}_{Q_j}}{1 - E'^2_0} \right) \frac{2p' \cdot q'_j + 2E'_0 \delta E'}{1 - E'^2_0} \psi_0 \]
\[ + \sum_{j=1}^{3} \hat{T}_{Q_j}^T \frac{\delta E'I + \sigma_0 \cdot p' \hat{T}_{Q_j}}{1 - E'^2_0} \psi_0 \]

Using the identities in Eq. (M10) as well as
\[ \sum_{j=1}^{3} \hat{T}_{Q_j}^T (\sigma_0 \cdot q'_j)(2p' \cdot q'_j) \hat{T}_{Q_j} = -3\lambda^2 w_1^2 \sigma_0 \cdot p' + 3\lambda^2 w_0^2 \sigma_{-2\phi_0} \cdot p' \]
\[ \sum_{j=1}^{3} \hat{T}_{Q_j}^T (2p' \cdot q'_j) \hat{T}_{Q_j} = 6\lambda^2 w_0 w_1 \sigma_{-\phi_0 - \pi/2} \cdot p' \] \hspace{1cm} (M17)
\[ \sum_{j=1}^{3} \hat{T}_{Q_j}^T (\sigma_0 \cdot p') \hat{T}_{Q_j} = 3\lambda^2 w_0^2 \sigma_{-2\phi_0} \cdot p', \]

The above equations are...
Eq. (M16) becomes
\[
\left(1 - \frac{2E_0'^3}{1 - E_0'^2} + \frac{3\lambda^2(w_0^2 + w_1^2)}{1 - E_0'^2}\right)\delta E'I + \left(-1 + \frac{3\lambda^2w_0^2}{1 - E_0'^2}\right)\sigma_0 \cdot p' + \frac{E_0'}{1 - E_0'^2}(6\lambda^2w_0w_1\sigma - \phi_0 - \pi/2 \cdot p')\delta E'I = 0. \tag{M18}
\]

We are interested in the conditions under which the terms proportional to \(p'\) in Eq. (M18) vanish so that \(\delta E'I = 0\) to first order in \(|p'|\). If \(E_0' = 0\), this condition is equivalent to \(3\lambda^2w_0^2 = 1\) or
\[
\lambda = \pm \frac{1}{|w_1|\sqrt{3}}. \tag{M19}
\]

Since \(E_0' = 0\) when \(w_0 = 0\) or \(\phi_0 = 0\), we recognize this as the magic angle condition identified in Refs. [3, 80], which is realizable in small angle TBG. However, there is another solution with \(\phi_0 = \pm \pi/2\) and
\[
\frac{3\lambda^2w_1^2}{1 - E_0'^2} = 1 \pm \frac{E_0'}{1 - E_0'^2}6\lambda^2w_0w_1 \tag{M20}
\]
or equivalently
\[
E_0'^2 \pm 6\lambda^2w_0w_1E_0' + 3\lambda^2w_1^2 - 1 = 0. \tag{M21}
\]

By Eq. (M12), \(E_0'\) also satisfies
\[
E_0'^3 - E_0'[1 + 3\lambda^2(w_0^2 + w_1^2)] \pm 6\lambda^2w_0w_1 = 0 \tag{M22}
\]
so we need to find when these two equations have a common solution for \(E_0'\) in the interval \((-1, 1)\). Assuming \(|w_0| \neq |w_1|\), we can take the approximation \(E_0'^3 \approx 0\) so that Eqs. (M21) and (M22) become
\[
27w_1^2(w_1^4 - 2w_0^2w_1^2 - 3w_0^4)\lambda^6 + 9(w_1^4 - w_0^4)\lambda^4 - 3(w_1^2 + 2w_0^2)\lambda^2 - 1 = 0. \tag{M23}
\]
It is easy to see that this equation has real solutions for \(\lambda\) if and only if \(|w_0| < |w_1|\).

We conclude that the magic angle conditions are Eq. (M19) when either \(w_0 = 0\) or \(\phi_0 = 0\), and Eq. (M23) when \(\phi_0 = \pm \pi/2\) and \(|w_0| < |w_1|\).

N. Additional moiré band structure plots

Figs. 14 to 17 show some additional moiré band structure plots (see captions for details).
(a) $(m, n) = (7, 3)$, $(\theta_0 \approx 27.8^\circ)$

(b) $(m, n) = (4, 3)$, $(\theta_0 \approx 46.8^\circ)$

(c) $(m, n) = (11, 3)$, $(\theta_0 \approx 17.9^\circ)$

(d) $(m, n) = (11, 9)$, $(\theta_0 \approx 50.6^\circ)$

FIG. 14. Moiré band structures at the first magic angle $\delta \theta = \delta \theta_{\text{magic}}$ near the latter four $(m, n)$ commensurate configurations in Tab. II, computed with Hamiltonian in Eq. (62). The horizontal axis follows a moiré quasi-momentum trajectory $\Gamma_M \to K_M \to \Gamma_M \to -M_M \to -K_M$ (note that $-K_M$ is equivalent to $K'_M$). The two bands nearest charge neutrality are shown in blue and red.

FIG. 15. Moiré band structures at the first magic manifold (angle) $\alpha^{-1} \approx \sqrt{3}$ at four different small $\phi_0$ in the model of Eq. (68), with $w_0/w_1 = 0.8$ and $w_2 = 0$. The horizontal axis follows a moiré quasi-momentum trajectory $\Gamma_M \to K_M \to M_M \to \Gamma_M \to -M_M \to -K_M$ (note that $-K_M$ is equivalent to $K'_M$). The two bands nearest charge neutrality are shown in blue and red.
FIG. 16. Moiré band structures with various parameters $w_0/w_1$ and $\alpha^{-1}$ located in the hyper-magic manifold (the three dark lines in Fig. 8(c)) at $\phi_0 = \pi/2$ in Eq. (68), where many flat bands can be seen in each panel. The horizontal axis follows a moiré quasi-momentum trajectory $\Gamma_M \rightarrow K_M \rightarrow \mathcal{M}_M \rightarrow \Gamma_M \rightarrow -\mathcal{M}_M \rightarrow -K_M$ (note that $-K_M$ is equivalent to $K'_M$). The two bands nearest charge neutrality are shown in blue and red. Note that panels (i) and (j) are in the chiral limit $w_0 = 0$ so that $\phi_0$ can take any real value and does not affect the band structure. The $\alpha^{-1}$ value of panel (i) and (j) correspond to the second and third magic angles in the chiral limit, respectively.
FIG. 17. Zoomed plots of a few examples of moiré band structures near charge neutrality, where the blue and red lines are the lowest conduction band and the lowest valence band, respectively. The horizontal axis is along the quasi-momentum trajectory $\Gamma_M \rightarrow K_M \rightarrow M_M \rightarrow \Gamma_M \rightarrow -M_M \rightarrow -K_M$ (note that $-K_M$ is equivalent to $K'_M$). (a)-(c) shows the gap closing transition between the lowest two bands and the remote bands (black) around the crossing of the upper two dark lines in the hyper-magic manifold (Fig. 8(c)), which changes the topology of the lowest two bands at charge neutrality from topological in (a) to trivial in (b). (d)-(f) shows a band inversion transition in the lowest dark line in the hyper-magic manifold: in panel (d), the lowest two moiré bands at charge neutrality become 2 of a group of 3 connected Kagome-like bands. In contrast, in panel (f), the lowest two moiré bands at charge neutrality are gapped from the remote bands.