Existence of the first magic angle for the chiral model of bilayer graphene

Alexander B. Watson[1, a)] and Mitchell Luskin[1, b)]

School of Mathematics, University of Minnesota Twin Cities

(Dated: 15 April 2021)

We consider the chiral model of twisted bilayer graphene introduced by Tarnopolsky-Kruchkov-Vishwanath (TKV). TKV have proved that for inverse twist angles α such that the effective Fermi velocity at the moiré K point vanishes, the chiral model has a perfectly flat band at zero energy over the whole Brillouin zone. By a formal expansion, TKV found that the Fermi velocity vanishes at $\alpha \approx .586$. In this work we prove the Fermi velocity vanishes at $\alpha \approx .586$, and put rigorous minimum and maximum bounds on the location of this zero, by rigorously justifying TKV's formal expansion of the Fermi velocity over a sufficiently large interval of α values. The idea of the proof is to project the TKV Hamiltonian onto a finite dimensional subspace, and then expand the Fermi velocity in terms of explicitly computable linear combinations of modes in the subspace, while controlling the error. The proof relies on two assumptions which can be checked numerically: a bound below on the smallest eigenvalue of a positive semi-definite, Hermitian 81×81 matrix which is essentially the square of the projected Hamiltonian, and an assumption on the validity of the negative value of a real 18th order polynomial approximating the numerator of the Fermi velocity when evaluated at a specific value of α. Since these assumptions can be verified up to high precision using standard numerical methods, together with TKV's work our result proves existence of at least one perfectly flat band of the chiral model.

a) watso860@umn.edu

b) luskin@umn.edu

I. INTRODUCTION

A. Outline

Twisted bilayer graphene (TBG) is formed by stacking one layer of graphene on top of another in such a way that the Bravais lattices of the layers are twisted relative to each other. For generic twist angles, the atomic lattices will be incommensurate so that the resulting structure will not have periodic structure. Bistritzer-MacDonald (BM)[1] have introduced an approximate model (BM model) for the electronic states of TBG which is periodic over the scale of the bilayer moiré pattern, where the twist angle enters as a parameter. Using this model, BM showed that the Fermi velocity, the velocity of electrons at the Fermi level, vanishes at particular twist angles known as "magic angles." The largest of these angles, known as the first magic angle, is at $\theta \approx 1.1$ degrees. Numerical computations on the BM model show the stronger result that at magic angles the Bloch band of the BM model at zero energy is approximately flat *over the whole Brillouin zone*[1,2]. The flatness of the zero energy Bloch band is thought to be a critical ingredient for recently observed superconductivity of TBG[3], although the precise mechanism for superconductivity in TBG is not yet settled.

Aiming at a simplified model which explains the nearly-flat band of TBG, Tarnopolsky-Kruchkov-Vishwanath (TKV)[4] have introduced a simplification of the BM model which has an additional "chiral" symmetry, known as the chiral model. TKV showed analytically that at magic angles (of the chiral model, still defined by vanishing of the Fermi velocity), the chiral model has *exactly* flat bands over the whole Brillouin zone. Using a formal perturbation theory (for the chiral model the natural parameter is the reciprocal of twist angle up to a constant) TKV have derived approximate values for the magic angles of the chiral model. It is worth noting that the first magic angles of the chiral model and the BM model are nearby, but the higher magic angles are not very close. Becker et al.[5] have introduced a spectral characterization of magic angles of the TKV model where the role of a non-normal operator is emphasized (the operator D^α appearing in (II.1)).

In this work we study the chiral model introduced by TKV and consider the problem of (1) rigorously proving existence of the first magic angle and (2) putting error bounds on its value. We do this by justifying the formal perturbation theory of TKV to make a rigorous expansion of the Fermi velocity to high enough order so that we can prove existence of a zero.

By numerically verifying that the resulting expansion attains a negative value (Assumption II.1), we obtain existence of the magic angle (Theorem II.2). By computing numerical values of the zero at extreme values of the error, we obtain non-trivial maximum and minimum possible values of the magic angle.

The proof of validity of the expansion is challenging because the reciprocal of the twist angle at the zero of the Fermi velocity is large relative to the spectral gap of the Hamiltonian, which means that the magic angle is outside of the range of validity of naïve perturbation theory of a simple eigenvalue. To overcome this difficulty, we start by representing the chiral model Hamiltonian in a basis which takes full advantage of model symmetries. Then, using a rigorous bound on the high frequency components of the error, we reduce the error analysis to analysis of the eigenvalues of the chiral model projected onto finitely many low frequencies. The error analysis (Theorem II.1) is then complete under an assumption on the eigenvalues of the projected chiral model which can easily be checked numerically (Assumption IV.1).

II. STATEMENT OF RESULTS

A. Tarnopolsky-Kruchkov-Vishwanath's chiral model

The chiral model, like the Bistritzer-MacDonald model (B-M model) from which it is derived, is a formal continuum approximation to the atomistic tight-binding model of twisted bilayer graphene. The BM and chiral models aim to capture physics over the length-scale of the bilayer moiré pattern, which is, for small twist angles, much longer than the length-scale of the individual graphene layer lattices. Crucially, even when the graphene layers are incommensurate so that the bilayer is aperiodic on the atomistic scale, the chiral model and BM model are periodic (up to phases) with respect to the moiré lattice, so that they can be analyzed via Bloch theory.

We define the moiré lattice to be the Bravais lattice

$$\Lambda = \left\{ m_1 \boldsymbol{a}_1 + m_2 \boldsymbol{a}_2 : (m_1, m_2) \in \mathbb{Z}^2 \right\}$$

generated by the moiré lattice vectors

$$\boldsymbol{a}_1 = \frac{2\pi}{3} \left(\sqrt{3}, 1 \right), \quad \boldsymbol{a}_2 = \frac{2\pi}{3} \left(-\sqrt{3}, 1 \right),$$

and denote a fundamental cell of the moiré lattice by Ω. The moiré reciprocal lattice is the Bravais lattice

$$\Lambda^* = \left\{ n_1 \boldsymbol{b}_1 + n_2 \boldsymbol{b}_2 : (n_1, n_2) \in \mathbb{Z}^2 \right\}$$

generated by the moiré reciprocal lattice vectors defined by $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$, given explicitly by

$$\boldsymbol{b}_1 = \frac{1}{2}\left(\sqrt{3}, 3\right), \quad \boldsymbol{b}_2 = \frac{1}{2}\left(-\sqrt{3}, 3\right).$$

We define $\boldsymbol{q}_1 = \left(0, -1\right)$, which is the (re-scaled) difference of the K points (Dirac points) of each layer, and

$$\boldsymbol{q}_1 = \left(0, -1\right), \quad \boldsymbol{q}_2 = \boldsymbol{q}_1 + \boldsymbol{b}_1 = \frac{1}{2}\left(\sqrt{3}, 1\right), \quad \boldsymbol{q}_3 = \boldsymbol{q}_1 + \boldsymbol{b}_2 = \frac{1}{2}\left(-\sqrt{3}, 1\right).$$

We write Ω^* for a fundamental cell of the moiré reciprocal lattice, and refer to such a cell as the Brillouin zone.

Let $\phi := \frac{2\pi}{3}$. Tarnopolsky-Kruchkov-Vishwanath's chiral Hamiltonian is defined as

$$H^\alpha = \begin{pmatrix} 0 & D^{\alpha\dagger} \\ D^\alpha & 0 \end{pmatrix}, \quad D^\alpha = \begin{pmatrix} -2i\overline{\partial} & \alpha U(\boldsymbol{r}) \\ \alpha U(-\boldsymbol{r}) & -2i\overline{\partial} \end{pmatrix}, \tag{II.1}$$

where $\overline{\partial} = \frac{1}{2}(\partial_x + i\partial_y)$, $U(\boldsymbol{r}) = e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{i\phi}e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}} + e^{-i\phi}e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}$, $\dagger$ denotes the adjoint (Hermitian transpose), and α is a real parameter which we will take to be positive $\alpha \geq 0$ throughout (see (II.3)) The chiral Hamiltonian H^α is an unbounded operator on $\mathcal{H} = L^2(\mathbb{R}^2; \mathbb{C}^4)$ with domain $H^1(\mathbb{R}^2; \mathbb{C}^4)$. We will write functions in $\mathcal{H}$ as

$$\psi(\boldsymbol{r}) = \left(\psi_1^A(\boldsymbol{r}), \psi_2^A(\boldsymbol{r}), \psi_1^B(\boldsymbol{r}), \psi_2^B(\boldsymbol{r})\right), \tag{II.2}$$

where $\psi_\tau^\sigma(\boldsymbol{r})$ represents the electron density near to the K point (in momentum space) on sublattice σ and on layer τ. The diagonal terms of D^α arise from Taylor expanding the single layer graphene dispersion relation about the K point of each layer, while the off-diagonal terms of D^α couple the A and B sublattices of layers 1 and 2. The chiral model is identical to the BM model except that inter-layer coupling between sublattices of the same type is turned off in the chiral model. The precise form of the interlayer coupling potential $U(\boldsymbol{r})$ can be derived under quite general assumptions on the real space interlayer hopping[1,6]. The parameter α is, up to unimportant constants, the ratio

$$\alpha \sim \frac{\text{interlayer hopping strength between } A \text{ and } B \text{ sublattices}}{\text{twist angle}}. \tag{II.3}$$

Although the limit $\alpha \to 0$ can be thought of as the limit of vanishing interlayer hopping strength at fixed twist, it is physically more interesting to view the limit as modeling decreasing twist angle at a fixed interlayer hopping strength.

B. Rigorous justification of TKV's formal expansion of the Fermi velocity and proof of existence of first magic angle

Bistritzer and MacDonald studied the effective Fermi velocity of electrons in twisted bilayer graphene modeled by the BM model, and computed values of the twist angle such that the Fermi velocity vanishes, which they called "magic angles." One can similarly define an effective Fermi velocity for the chiral model, and refer to values of α such that the Fermi velocity vanishes as "magic angles" (although technically α is related to the reciprocal of the twist angle (II.3)).

TKV proved the remarkable result that, at magic angles, the chiral model has a perfectly flat Bloch band at zero energy. Let L^2_K denote the L^2 space on a single moiré cell Ω with moiré K point Bloch boundary conditions. The starting point of TKV's proof is an expression for the Fermi velocity as a function of α, $v(\alpha)$, as a functional of one of the Bloch eigenfunctions, $\psi^\alpha(\boldsymbol{r}) \in L^2_K$, of H^α:

$$v(\alpha) := \frac{|\langle \psi^{\alpha *}(-\boldsymbol{r}) | \psi^\alpha(\boldsymbol{r}) \rangle|}{|\langle \psi^\alpha(\boldsymbol{r}) | \psi^\alpha(\boldsymbol{r}) \rangle|}, \tag{II.4}$$

where $\langle . | . \rangle$ denotes the L^2_K inner product. We give precise definitions of L^2_K, $\psi^\alpha(\boldsymbol{r})$, and $v(\alpha)$ in Definition III.2, Proposition III.5, and Definition III.3, respectively. We prove the denominator of (II.4) is non-zero for all α in Proposition III.7. We give a systematic formal derivation of why (II.4) is the effective Fermi velocity at the moiré K point in Appendix A. To complete the proof, TKV showed that zeros of $v(\alpha)$ imply zeros of $\psi^\alpha(\boldsymbol{r})$ at special "stacking points" of Ω, and that such zeros of $\psi^\alpha(\boldsymbol{r})$ allow for Bloch eigenfunctions with zero energy to be constructed for all $\boldsymbol{k}$ in the moiré Brillouin zone.

To derive approximate values for magic angles, TKV computed a formal perturbation series approximation of $\psi^\alpha(\boldsymbol{r})$:

$$\psi^\alpha(\boldsymbol{r}) = \Psi^0(\boldsymbol{r}) + \alpha \Psi^1(\boldsymbol{r}) + ... \tag{II.5}$$

and then substituted this expression into the functional for $v(\alpha)$ to obtain an expansion of

$v(\alpha)$ in powers of α:

$$v(\alpha) = \frac{1 - 3\alpha^2 + \alpha^4 - \frac{111}{49}\alpha^6 + \frac{143}{294}\alpha^8 + ...}{1 + 3\alpha^2 + 2\alpha^4 + \frac{6}{7}\alpha^6 + \frac{107}{98}\alpha^8 + ...}. \tag{II.6}$$

By setting $v(\alpha) = 0$ one obtains an approximation for the smallest magic angle: $\alpha \approx .586$.

Although TKV proved that flat bands occur at magic angles, they did not prove the existence of magic angles, and hence they did not prove the existence of flat bands. The contribution of the present work is to prove rigorous estimates on the error in the approximation (II.5) which are sufficiently high order and precise that, once substituted into (II.4), they suffice to rigorously prove the existence of a zero of $v(\alpha)$, and hence, via TKV's proof, the existence of at least one perfectly flat band.

The first main theorem we will prove, roughly stated, is the following. See Theorem IV.1 for the more precise statement. The theorem relies on an assumption about the smallest eigenvalue of a 81×81 positive semi-definite Hermitian matrix which must be checked numerically, see Assumption IV.1.

Theorem II.1. *The K point Bloch function $\psi^\alpha(\boldsymbol{r})$ satisfies*

$$\psi^\alpha(\boldsymbol{r}) = \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) + \eta^\alpha(\boldsymbol{r}) \tag{II.7}$$

where $\eta^\alpha(\boldsymbol{r}) \perp \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r})$ with respect to the L^2_K inner product, and

$$\|\eta^\alpha\|_{L^2_K} \leq \frac{3\alpha^9}{15 - 20\alpha} \quad \textit{for all} \quad 0 \leq \alpha \leq \frac{7}{10}. \tag{II.8}$$

The functions $\Psi^n(\boldsymbol{r})$ for $1 \leq n \leq 8$ are derived recursively: see Appendix C. We stop at 8th order in the expansion because this is the minimal order such that we can guarantee existence of a zero of $v(\alpha)$, but the functions $\Psi^n(\boldsymbol{r})$ are well defined by a recursive procedure for arbitrary positive integers n, see Proposition IV.1.

Substituting (II.7) into the functional for the Fermi velocity (II.4) and using $\eta^\alpha(\boldsymbol{r}) \perp \sum_{n=1}^{8} \alpha^n \Psi^n(\boldsymbol{r})$ we find

$$v(\alpha) = \frac{v_{\mathcal{N}}(\alpha)}{v_{\mathcal{D}}(\alpha)} \tag{II.9}$$

where

$$v_{\mathcal{N}}(\alpha) := \left\langle \sum_{n=0}^{8} \alpha^n \Psi^{n*}(-\boldsymbol{r}) \middle| \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle + \left\langle \eta^{\alpha*}(-\boldsymbol{r}) \middle| \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle + \left\langle \sum_{n=0}^{8} \Psi^{n*}(-\boldsymbol{r}) \middle| \eta^{\alpha}(\boldsymbol{r}) \right\rangle + \langle \eta^{\alpha*}(-\boldsymbol{r}) | \, \eta^{\alpha}(\boldsymbol{r}) \rangle \,, \tag{II.10}$$

and

$$v_{\mathcal{D}}(\alpha) := \left\langle \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \middle| \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle + \langle \eta^{\alpha}(\boldsymbol{r}) | \, \eta^{\alpha}(\boldsymbol{r}) \rangle \,.$$

where $\langle . | . \rangle$ denotes the L^2_K inner product and $\eta^\alpha(\boldsymbol{r})$ satisfies (II.8). The following is a straightforward calculation.

Proposition II.1. *The following identities hold:*

$$\left\langle \sum_{n=0}^{8} \alpha^n \Psi^{n*}(-\boldsymbol{r}) \middle| \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle = 1 - 3\alpha^2 + \alpha^4 - \frac{111}{49}\alpha^6 + \frac{143}{294}\alpha^8 - \frac{7536933}{11957764}\alpha^{10} + \frac{4598172331}{47460365316}\alpha^{12} - \frac{30028809212865451}{520327364608478700}\alpha^{14} + \frac{49750141858992227}{12487856750603488800}\alpha^{16}, \tag{II.11}$$

$$\left\langle \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \middle| \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle = 1 + 3\alpha^2 + 2\alpha^4 + \frac{6}{7}\alpha^6 + \frac{107}{98}\alpha^8 + \frac{5119}{48412}\alpha^{10} + \frac{62026511}{356844852}\alpha^{12} + \frac{355691470247}{113410497953025}\alpha^{14} + \frac{2481663780475871}{337509641908202400}\alpha^{16}. \tag{II.12}$$

We prove Proposition II.1 in Appendix F. Naïvely, the expansions (II.11) and (II.12) approximate the formal infinite series expansions of $\langle \sum_{n=0}^{\infty} \alpha^n \Psi^{n*}(-\boldsymbol{r}) | \sum_{n=0}^{\infty} \alpha^n \Psi^n(\boldsymbol{r}) \rangle$ and $\langle \sum_{n=0}^{\infty} \alpha^n \Psi^{n}(\boldsymbol{r}) | \sum_{n=0}^{\infty} \alpha^n \Psi^n(\boldsymbol{r}) \rangle$ up to terms of order α^9. We prove in Proposition F.2 that, because of some simplifications, expansions (II.11) and (II.12) agree with the infinite series up to terms of order α^{10}.

We are now in a position to state and prove our second result. This result also relies on an assumption which must be checked numerically: that an 18th order polynomial in α attains a negative value, see Assumption II.1.

Theorem II.2. *There exist positive numbers α_{min} and α_{max} such that the Fermi velocity $v(\alpha)$ defined by* (II.4) *has a zero α^* between $\alpha_{min} \leq \alpha^* \leq \alpha_{max}$.*

Proof. Equation (II.10) and Cauchy-Schwarz imply that

$$\left|v_{\mathcal{N}}(\alpha) - \left\langle \sum_{n=0}^{8} \alpha^n \Psi^{n*}(-\boldsymbol{r}) \middle| \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle\right| \leq 2\|\eta^\alpha(\boldsymbol{r})\| \sum_{n=0}^{8} \alpha^n \|\Psi^n(\boldsymbol{r})\| + \|\eta^\alpha(\boldsymbol{r})\|^2.$$

Using Theorem II.1 and Proposition C.3, It follows that to prove that $v(\alpha)$ has a zero it suffices to check that the upper bound on the numerator of (II.9),

$$\begin{aligned} &1 - 3\alpha^2 + \alpha^4 - \frac{111}{49}\alpha^6 + \frac{143}{294}\alpha^8 - \frac{7536933}{11957764}\alpha^{10} \\ &+ \frac{4598172331}{47460365316}\alpha^{12} - \frac{30028809212865451}{520327364608478700}\alpha^{14} + \frac{49750141858992227}{1248785675060348800}\alpha^{16} \\ &+ \mathcal{E}(\alpha), \end{aligned} \tag{II.13}$$

where

$$\begin{aligned} \mathcal{E}(\alpha) := \frac{6\alpha^9}{15-20\alpha} \Bigg(& 1 + \sqrt{3}\alpha + \sqrt{2}\alpha^2 + \frac{\sqrt{14}}{7}\alpha^3 + \frac{\sqrt{258}}{42}\alpha^4 + \frac{\sqrt{1968837}}{3458}\alpha^5 \\ & + \frac{\sqrt{106525799}}{31122}\alpha^6 + \frac{2\sqrt{2129312323981473}}{624696345}\alpha^7 + \frac{\sqrt{183643119755214454}}{4997570760}\alpha^8 \Bigg) \\ & + \frac{9\alpha^{18}}{(15-20\alpha)^2}, \end{aligned}$$

where we use Proposition C.3 to calculate the term in brackets, has a zero for positive α. Noting that, upon multiplying by $(15-20\alpha)^2$, (II.13) is an 18th order polynomial in α, it is easy to verify numerically that this holds, see Figure II.1. We make this precise as an assumption.

Assumption II.1. *Expression* (II.13)*, or equivalently the 18th order polynomial obtained by multiplying* (II.13) *by* $(15-20\alpha)^2$*, has a zero for* $0 < \alpha < \frac{3}{4}$.

Note that Assumption II.1 can be checked by merely evaluating (II.13) at different values of α and finding a negative value. Specifically, evaluating using double-precision we find that at $\alpha = .646$, (II.13) attains the negative value -0.068430 (five significant figures). The result of a forward error analysis for the round-off error and the error in the computation of the square roots would then give a negative upper bound for the value of the polynomial and rigorously confirm Assumption II.1.

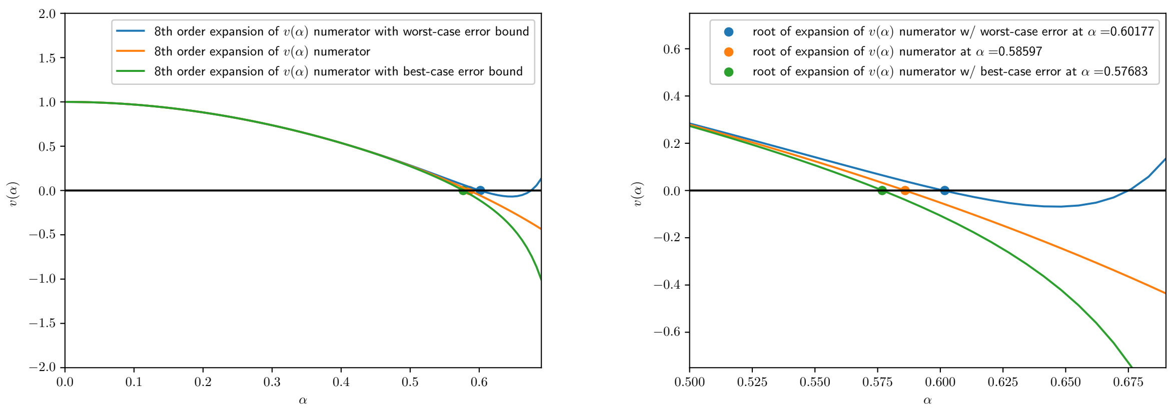

FIG. II.1. At left, plot of the numerator $v_{\mathcal{N}}(\alpha)$ of the Fermi velocity approximated by the 8th order TKV expansion (II.6) (orange), and of 8th order expansions with worst-case (II.13) (blue) and best-case (II.14) (green) errors. At right, detail showing roots of these functions near to $\alpha = \frac{1}{\sqrt{3}} \approx .57735$ (five significant figures).

We denote the zero of (II.13) by α_{max}. Existence of such a zero implies the existence of a zero, which we denote by α_{min}, of the expression obtained by bounding the error below:

$$\begin{aligned} &1 - 3\alpha^2 + \alpha^4 - \frac{111}{49}\alpha^6 + \frac{143}{294}\alpha^8 - \frac{7536933}{11957764}\alpha^{10} \\ &\quad + \frac{4598172331}{47460365316}\alpha^{12} - \frac{300288092128654 51}{520327364608478700}\alpha^{14} + \frac{497501418589922 27}{1248785675060348880 0}\alpha^{16} \\ &\quad - \mathcal{E}(\alpha). \end{aligned} \tag{II.14}$$

The result now follows. □

Numerical computation of the zeros α_{min} and α_{max} gives $\alpha_{min} = 0.57683$ (5sf) and $\alpha_{max} = 0.60177$ (5sf) respectively, where (5sf) is an abbreviation for (five significant figures), see Figure II.1.

Our results rely on numerical computation in two places, specifically to verify Assumptions IV.1 and II.1. These assumptions can be checked with standard algorithms.

Using Proposition C.1 and the package Sympy[7] for symbolic computation we can compute the formal expansion of $v(\alpha)$ up to arbitrarily high order in α. In particular, we find the higher-order terms in the expansion (II.6) to be

$$v(\alpha) = \frac{1 - 3\alpha^2 + \alpha^4 - \frac{111}{49}\alpha^6 + \frac{143}{294}\alpha^8 - \frac{10227257}{11957764}\alpha^{10} + \frac{6881137015}{47460365316}\alpha^{12} - \frac{130055941435858531}{520327364608478700}\alpha^{14} + \ldots}{1 + 3\alpha^2 + 2\alpha^4 + \frac{6}{7}\alpha^6 + \frac{107}{98}\alpha^8 + \frac{16011}{48412}\alpha^{10} + \frac{134058653}{356844852}\alpha^{12} + \frac{26407145691649}{226820995906050}\alpha^{14} + \ldots}.$$

Truncating after order α^{14} and setting the numerator equal to zero yields the estimate $\alpha = 0.5856640$ (7sf) for the first magic angle.

C. Structure of paper

We review the symmetries, Bloch theory, and symmetry-protected zero modes of TKV's chiral model in Section III. We prove Theorem II.1 in Section IV, postponing most details of the proofs to the appendices. In Appendix A we show why (II.4) corresponds to the effective Fermi velocity at the moiré K point. In Appendix B, we construct an orthonormal basis, which we refer to as the chiral basis, which allows for efficient computation and analysis of TKV's formal expansion. We re-derive TKV's formal expansions in Appendix C. We give details of the proof of Theorem II.1 in Appendices D and E. We prove Proposition II.1 in Appendix F. In the supplementary material, we list the basis functions of the subspace onto which we project the TKV Hamiltonian, give the explicit forms of the higher-order corrections in the expansion (II.7), and present a derivation of the TKV Hamiltonian from the Bistritzer-MacDonald model.

III. SYMMETRIES, BLOCH THEORY, AND ZERO MODES OF TKV'S CHIRAL MODEL

A. Symmetries of the TKV model

Recall that $\phi = \frac{2\pi}{3}$ and let R_ϕ denote the matrix which rotates vectors counter-clockwise by ϕ, i.e.,

$$R_\phi = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}.$$

We define

Definition III.1. *For any $\boldsymbol{v} \in \Lambda$ we define a phase-shifted translation operator acting on functions $f(\boldsymbol{r}) \in \mathcal{H}$ by*

$$\tau_{\boldsymbol{v}} f(\boldsymbol{r}) := \text{diag}\left(1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}, 1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}\right) \tilde{\tau}_{\boldsymbol{v}} f(\boldsymbol{r}), \quad \tilde{\tau}_{\boldsymbol{v}} f(\boldsymbol{r}) = f(\boldsymbol{r}+\boldsymbol{v}). \tag{III.1}$$

We define a phase-shifted version of the operator which rotates functions $f(\boldsymbol{r}) \in \mathcal{H}$ clockwise *by ϕ by*

$$\mathcal{R}f(\boldsymbol{r}) := \operatorname{diag}\left(1, 1, e^{-i\phi}, e^{-i\phi}\right) \tilde{\mathcal{R}}f(\boldsymbol{r}), \quad \tilde{\mathcal{R}}f(\boldsymbol{r}) = f(R_\phi \boldsymbol{r}). \tag{III.2}$$

For any $f(\boldsymbol{r}) \in \mathcal{H}$ we finally define the "chiral" symmetry operator

$$\mathcal{S}f(\boldsymbol{r}) := \operatorname{diag}(1, 1, -1, -1) f(\boldsymbol{r}). \tag{III.3}$$

We then have the following.

Proposition III.1. *The operators* (III.1) *and* (III.2) *are symmetries in the sense that*

$$[H^\alpha, \tau_{\boldsymbol{v}}] = H^\alpha \tau_{\boldsymbol{v}} - \tau_{\boldsymbol{v}} H^\alpha = 0 \tag{III.4}$$

for all moiré lattice vectors $\boldsymbol{v} \in \Lambda$,

$$[H^\alpha, \mathcal{R}] = H^\alpha \mathcal{R} - \mathcal{R} H^\alpha = 0,$$

and the operator (III.3) *is a "chiral" symmetry in the sense that*

$$\{H^\alpha, \mathcal{S}\} = H^\alpha \mathcal{S} + \mathcal{S} H^\alpha = 0. \tag{III.5}$$

Proof. The first claim is a direct calculation using the facts that for any $\boldsymbol{v} \in \Lambda$

$$\tilde{\tau}_{-\boldsymbol{v}} U(\boldsymbol{r}) \tilde{\tau}_{\boldsymbol{v}} = e^{-i\boldsymbol{q}_1 \cdot \boldsymbol{v}} U(\boldsymbol{r}), \quad \tilde{\tau}_{-\boldsymbol{v}} \overline{\partial} \tilde{\tau}_{\boldsymbol{v}} = \overline{\partial}.$$

The second claim is a direct calculation using the facts that

$$\tilde{\mathcal{R}}^{-1} U(\boldsymbol{r}) \tilde{\mathcal{R}} = e^{-i\phi} U(\boldsymbol{r}), \quad \tilde{\mathcal{R}}^{-1} \overline{\partial} \tilde{\mathcal{R}} = e^{-i\phi} \overline{\partial}.$$

The final claim is trivial to check. $\square$

The "chiral" symmetry (III.5) implies that the spectrum of H^α is symmetric about zero, because

$$H^\alpha \psi = E\psi \iff H^\alpha \mathcal{S}\psi = -E\mathcal{S}\psi.$$

The same calculation implies that zero modes of H^α can always be chosen without loss of generality to be eigenfunctions of $\mathcal{S}$.

B. Bloch theory for the TKV Hamiltonian

We now want to reduce the eigenvalue problem for H^α using the symmetries just introduced. The symmetry (III.4) means that eigenfunctions of H^α can be chosen without loss of generality to be simultaneous eigenfunctions of $\tau_{\boldsymbol{v}}$ for all $\boldsymbol{v} \in \Lambda$. It therefore suffices to seek solutions of

$$H^\alpha \psi = E\psi$$

for $\boldsymbol{r}$ in a fundamental cell $\Omega := \mathbb{R}^2/\Lambda$ of the moiré lattice in the symmetry-restricted spaces

$$L^2_{\boldsymbol{k}} := \left\{ f(\boldsymbol{r}) \in L^2(\Omega; \mathbb{C}^4) : f(\boldsymbol{r}+\boldsymbol{v}) = e^{i\boldsymbol{k}\cdot\boldsymbol{v}} \operatorname{diag}(1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}, 1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}) f(\boldsymbol{r}) \;\forall \boldsymbol{v} \in \Lambda \right\} \tag{III.6}$$

where $\boldsymbol{k}$ is known as the quasimomentum. Since $L^2_{\boldsymbol{k}+\boldsymbol{w}} = L^2_{\boldsymbol{k}}$ for any $\boldsymbol{w} \in \Lambda^*$, it suffices to restrict attention to $\boldsymbol{k}$ in a fundamental cell of Λ^* which we denote $\Omega^* := \mathbb{R}^2/\Lambda^*$ and refer to as the Brillouin zone.

We now claim the following.

Proposition III.2. *Let $f(\boldsymbol{r}) \in L^2_{\boldsymbol{k}}$. Then $\mathcal{R}f(\boldsymbol{r}) \in L^2_{R^*_\phi \boldsymbol{k}}$.*

Proof. By definition, for any $\boldsymbol{v} \in \Lambda$,

$$\mathcal{R}f(\boldsymbol{r}+\boldsymbol{v}) = \operatorname{diag}(1, 1, e^{-i\phi}, e^{-i\phi}) f(R_\phi \boldsymbol{r} + R_\phi \boldsymbol{v}).$$

By the definition of $L^2_{\boldsymbol{k}}$ we have

$$\mathcal{R}f(\boldsymbol{r}+\boldsymbol{v}) = e^{i(R^*_\phi \boldsymbol{k})\cdot\boldsymbol{v}} \operatorname{diag}(1, e^{i(R^*_\phi \boldsymbol{q}_1)\cdot\boldsymbol{v}}, 1, e^{i(R^*_\phi \boldsymbol{q}_1)\cdot\boldsymbol{v}}) \mathcal{R}f(\boldsymbol{r}).$$

The conclusion now follows from $R^*_\phi \boldsymbol{q}_1 = \boldsymbol{q}_1 + \boldsymbol{b}_2$ and $\boldsymbol{b}_2 \cdot \boldsymbol{v} = 0 \bmod 2\pi$ for all $\boldsymbol{v} \in \Lambda$. □

In particular, whenever $R^*_\phi \boldsymbol{k} = \boldsymbol{k} \bmod \Lambda^*$, we have $\mathcal{R}L^2_{\boldsymbol{k}} = L^2_{\boldsymbol{k}}$. Regarding such $\boldsymbol{k}$, the following is a simple calculation.

Proposition III.3. *The moiré K and K' points $\boldsymbol{k} = 0$ and $\boldsymbol{k} = -\boldsymbol{q}_1$, and the moiré Γ point $\boldsymbol{k} = \boldsymbol{q}_1 + \boldsymbol{b}_1$ satisfy $R^*_\phi \boldsymbol{k} = \boldsymbol{k} \bmod \Lambda^*$.*

The moiré K, K', and Γ points are shown in Figure III.1. Note that the moiré K, K', and Γ points should not be confused with the single layer K, K', and Γ points. The moiré K point corresponds to the K point of layer 1, while the moiré K' point corresponds to the

K point of layer 2. Interactions with the K' points of layers 1 and 2 are formally small for small twist angles and are hence ignored.

In this work we will be particularly interested in Bloch functions at the moiré K and K' points. We therefore define

Definition III.2.

$$L^2_K := L^2_{\mathbf{0}}, \quad L^2_{K'} := L^2_{-\boldsymbol{q}_1}.$$

Let $\omega = e^{i\phi}$. Since the spaces L^2_K and $L^2_{K'}$ are invariant under $\mathcal{R}$ they can be divided up into invariant subspaces corresponding to the eigenvalues of $\mathcal{R}$

$$L^2_K = L^2_{K,1} \oplus L^2_{K,\omega} \oplus L^2_{K,\omega^*}, \quad L^2_{K'} = L^2_{K',1} \oplus L^2_{K',\omega} \oplus L^2_{K',\omega^*},$$

where

$$L^2_{K,\sigma} := \left\{ f(\boldsymbol{r}) \in L^2_K : \mathcal{R} f(\boldsymbol{r}) = \sigma f(\boldsymbol{r}) \right\} \quad \sigma = 1, \omega, \omega^*$$

and $L^2_{K',\sigma}, \sigma = 1, \omega, \omega^*$, are defined similarly.

The following, which is trivial to prove, will be important for studying the zero modes of H^α.

Proposition III.4. *The operator $\mathcal{S}$ commutes with $\tau_{\boldsymbol{v}}$ and $\mathcal{R}$ and hence maps the $L^2_{K,\sigma}$ and $L^2_{K',\sigma}$ spaces to themselves for $\sigma = 1, \omega, \omega^*$.*

Since $\mathcal{S}$ has eigenvalues ± 1, we can define the spaces

$$L^2_{K,\sigma,\pm 1} = \left\{ f(\boldsymbol{r}) \in L^2_{K,\sigma} : \mathcal{S} f(\boldsymbol{r}) = \pm f(\boldsymbol{r}) \right\} \quad \sigma = 1, \omega, \omega^*$$

and spaces $L^2_{K',\sigma,\pm 1}, \sigma = 1, \omega, \omega^*$ similarly.

Remark III.1. *Note that $+1$ eigenspaces of $\mathcal{S}$ correspond to wave-functions which vanish in their third and fourth entries, which correspond, through* (II.2)*, to wave-functions supported only on A sites of the layers. Similarly, -1 eigenspaces of $\mathcal{S}$ correspond to wave-functions which vanish in their first and second entries, which are supported only on B sites of the layers.*

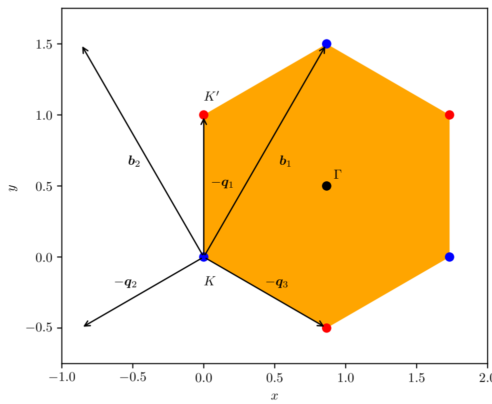

FIG. III.1. Diagram showing locations of moiré K (blue), K' (red), and Γ (black) points within the moiré Brillouin zone (orange).

C. Zero modes of the chiral model

We now want to investigate zero modes of H^α in detail. When $\alpha = 0$, there are exactly four zero modes given by $e_j(\boldsymbol{r}), j = 1, 2, 3, 4$ where $e_j(\boldsymbol{r})$ equals 1 in its jth entry and 0 in its other entries. It is easy to check that

$$e_1 \in L^2_{K,1}, \quad e_2 \in L^2_{K',1}, \quad e_3 \in L^2_{K,\omega^*}, \quad e_4 \in L^2_{K',\omega^*}, \tag{III.7}$$

and hence 0 is a simple eigenvalue of H^α when restricted to each of these subspaces. Recall that zero modes can always be chosen as eigenfunctions of $\mathcal{S}$, and indeed we have

$$e_1 \in L^2_{K,1,1}, \quad e_2 \in L^2_{K',1,1}, \quad e_3 \in L^2_{K,\omega^*,-1}, \quad e_4 \in L^2_{K',\omega^*,-1}.$$

We now claim that these zero modes persist for all α.

Proposition III.5. *There exist functions $\psi^\alpha(\boldsymbol{r})$ in each of the spaces $L^2_{K,1,1}$, $L^2_{K',1,1}$, $L^2_{K,\omega^*,-1}$, $L^2_{K',\omega^*,-1}$ such that $\psi^0(\boldsymbol{r})$ is as in* (III.7)*, $\alpha \mapsto \psi^\alpha(\boldsymbol{r})$ is analytic, and $H^\alpha \psi^\alpha(\boldsymbol{r}) = 0$ for all α. The dimension of* $\ker H^\alpha$ *restricted to each of the spaces $L^2_{K,1}$, $L^2_{K',1}$, L^2_{K,ω^*}, L^2_{K,ω^*} is always odd-dimensional.*

Proof. Since $\mathcal{S}$ preserves each of the spaces $L^2_{K,1}$, $L^2_{K',1}$, L^2_{K,ω^*}, L^2_{K,ω^*} and anti-commutes with H^α, the spectrum of H^α restricted to each space must be symmetric about 0 for all α. The result now follows from analyticity of the eigenvalues (note that the analytic choice of eigenvalue at a degeneracy may not respect eigenvalue ordering) and associated eigenprojections[8] of H^α as a function of α. It is clear from analyticity that the $\mathcal{S}$ eigenvalue of each zero mode cannot change. □

In this work we will restrict attention to the moiré K point, and especially the family $\psi^\alpha(\boldsymbol{r}) \in L^2_{K,1,1}$. We expect that our analysis would go through with only minor modifications if we considered instead the moiré K' point. The zero modes in $L^2_{K,1,1}$ and $L^2_{K,\omega^*,-1}$ are related by the following symmetry.

Proposition III.6. *Let $\psi^\alpha_1(\boldsymbol{r})$ and $\psi^\alpha_{-1}(\boldsymbol{r})$ denote the zero modes of H^α in the spaces $L^2_{K,1,1}$ and $L^2_{K,\omega^*,-1}$ respectively. Then $\psi^\alpha_1(\boldsymbol{r}) = (\Phi^\alpha(\boldsymbol{r}), 0)^\top$ where $\Phi^\alpha(\boldsymbol{r}) \in L^2(\Omega; \mathbb{C}^2)$, $\Phi^\alpha(\boldsymbol{r}+\boldsymbol{v}) = \text{diag}(1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}})\Phi^\alpha(\boldsymbol{r})$ for all $\boldsymbol{v} \in \Lambda$, $\Phi^\alpha(R_\phi \boldsymbol{r}) = \Phi^\alpha(\boldsymbol{r})$ and $\psi^\alpha_{-1}(\boldsymbol{r}) = (0, \Phi^{\alpha *}(-\boldsymbol{r}))^\top$.*

Proof. Since $\mathcal{S}\psi^\alpha_1(\boldsymbol{r}) = \psi^\alpha_1(\boldsymbol{r})$, the last two entries of $\psi^\alpha_1(\boldsymbol{r})$ must vanish, so we can write $\psi^\alpha_1(\boldsymbol{r}) = (\Phi^\alpha(\boldsymbol{r}), 0)^\top$. That $\Phi^\alpha(\boldsymbol{r})$ satisfies the stated symmetries follows immediately from $\psi^\alpha_1 \in L^2_{K,1}$. It is straightforward to check using the definitions of $\mathcal{R}$ and $\tau_{\boldsymbol{v}}$ that $(0, \Phi^{\alpha *}(-\boldsymbol{r}))^\top \in L^2_{K,\omega^*,-1}$. To see that $(0, \Phi^{\alpha *}(-\boldsymbol{r}))^\top$ is a zero mode, note that $\Phi^\alpha(\boldsymbol{r})$ satisfies $D^\alpha \Phi^\alpha(\boldsymbol{r}) = 0$, which implies that $D^{\alpha\dagger}\Phi^{\alpha *}(-\boldsymbol{r}) = 0$ by a simple manipulation. To see that $\psi^\alpha_2(\boldsymbol{r}) = (0, \Phi^{\alpha *}(-\boldsymbol{r}))^\top$ for all α, note that this clearly holds for $\alpha = 0$ and then must hold for all α by analyticity. □

In Appendix A we use Proposition III.6 to derive the effective Dirac operator with α-dependent Fermi velocity which controls the Bloch band structure in a neighborhood of the moiré K point. The Fermi velocity of the effective Dirac operator is given by the following. Note that we drop the subscript $+1$ when referring to the zero mode of H^α in $L^2_{K,1,1}$ since the zero mode of H^α in $L^2_{K,\omega^*,-1}$ plays no further role.

Definition III.3. *Let $\psi^\alpha(\boldsymbol{r}) \in L^2_{K,1,1}$ be as in Proposition III.5. Then we define*

$$v(\alpha) := \frac{|\,\langle \psi^{\alpha *}(-\boldsymbol{r}) |\, \psi^\alpha(\boldsymbol{r})\rangle\,|}{|\,\langle \psi^\alpha(\boldsymbol{r}) |\, \psi^\alpha(\boldsymbol{r})\rangle\,|} \tag{III.8}$$

where $\langle . | . \rangle$ denotes the L^2_K inner product.

Proposition III.7. *The denominator of* (II.4) *is non-zero for all α.*

Proof. Since $\langle \eta^\alpha(\boldsymbol{r}) |\, \eta^\alpha(\boldsymbol{r})\rangle \geq 0$, the result follows immediately from (II.12). □

IV. RIGOROUS JUSTIFICATION OF TKV'S EXPANSION OF THE FERMI VELOCITY

A. Alternative formulation of TKV's expansion

We now turn to approximating the zero mode $\psi^\alpha(\boldsymbol{r}) \in L^2_{K,1,1}$ by a series expansion in powers of α. We write $H^\alpha = H^0 + \alpha H^1$ and formally expand $\psi^\alpha(\boldsymbol{r})$ as a series

$$\psi^\alpha(\boldsymbol{r}) = \Psi^0(\boldsymbol{r}) + \alpha \Psi^1(\boldsymbol{r}) + ... \tag{IV.1}$$

where $H^0 \Psi^0(\boldsymbol{r}) = 0$, and

$$H^0 \Psi^n = -H^1 \Psi^{n-1} \tag{IV.2}$$

for all $n \geq 1$. To solve $H^0 \Psi^0(\boldsymbol{r}) = 0$ we take $\Psi^0(\boldsymbol{r}) = e_1(\boldsymbol{r})$. We prove the following in Appendix C.

Proposition IV.1. *Let P denote the projection operator in $L^2_{K,1}$ onto $e_1(\boldsymbol{r})$, and $P^\perp = I - P$. The sequence of equations* (IV.2) *has a unique solution such that $\Psi^n(\boldsymbol{r}) \in L^2_{K,1,1}$ for all $n \geq 0$ and $P\Psi^n(\boldsymbol{r}) = 0$ for all $n \geq 1$ given by $\Psi^0(\boldsymbol{r}) = e_1(\boldsymbol{r})$ and*

$$\Psi^n(\boldsymbol{r}) = -P^\perp (H^0)^{-1} P^\perp H^1 \Psi^{n-1}(\boldsymbol{r})$$

for each $n \geq 1$.

The expansion (IV.1) appears different from the series studied by TKV, since we work only with the self-adjoint operators H^0, H^1, and H^α rather than the non-self-adjoint operator D^α (defined in (II.1)). Since functions in $L^2_{K,1,1}$ vanish in their last two components, there is no practical difference. However, working with only self-adjoint operators allows us to use the spectral theorem, which greatly simplifies the error analysis. We compute the first eight terms in expansion (IV.1) in Proposition C.2 after developing some necessary machinery in Appendix B.

B. Rigorous error estimates for the expansion of the moiré K point Bloch function

In this section we explain the essential challenge in proving error estimates for the series (IV.1) and explain how we overcome this challenge. Our goal is to prove the following.

Theorem IV.1. *Let $\psi^\alpha(\boldsymbol{r}) \in L^2_{K,1,1}$ be as in Proposition III.5. Then*

$$\psi^\alpha(\boldsymbol{r}) = \sum_{n=1}^{8} \alpha^n \Psi^n(\boldsymbol{r}) + \eta^\alpha(\boldsymbol{r})$$

where $\eta^\alpha(\boldsymbol{r}) \perp \sum_{n=1}^{8} \alpha^n \Psi^n(\boldsymbol{r})$ with respect to the L^2_K inner product, and

$$\|\eta^\alpha\|_{L^2_{K,1}} \leq \frac{3\alpha^9}{15 - 20\alpha} \quad \textit{for all} \quad 0 \leq \alpha \leq \frac{7}{10}.$$

Proposition IV.1 guarantees that the series (IV.1) is well-defined up to arbitrarily many terms. A naïve bound on the growth of terms in the series comes from the following proposition.

Proposition IV.2. *The spectrum of H^0 in $L^2_{K,1}$ is*

$$\sigma_{L^2_{K,1}}(H^0) = \{\pm|\boldsymbol{G}|, \pm|\boldsymbol{q}_1 + \boldsymbol{G}| : \boldsymbol{G} \in \Lambda^*\}$$

and hence

$$\|P^\perp (H^0)^{-1} P^\perp\|_{L^2_{K,1} \to L^2_{K,1}} = 1. \tag{IV.3}$$

We also have

$$\|H^1\|_{L^2_{K,1} \to L^2_{K,1}} = 3. \tag{IV.4}$$

Proof. This proposition is a combination of Propositions B.2, B.4, and B.7, proved in Appendix B. □

Proposition IV.2 implies that $\|P^\perp (H^0)^{-1} P^\perp H^1\|_{L^2_{K,1} \to L^2_{K,1}} \leq 3$ which guarantees that the series (IV.1) converges in $L^2_{K,1}$ as long as $\alpha < \frac{1}{3}$. However, this restriction is too strong to prove that the Fermi velocity has a zero, which occurs at the larger value $\alpha \approx \frac{1}{\sqrt{3}}$. Of course, Proposition IV.2 establishes only the most pessimistic possible bound on Ψ^N, and this bound appears to be far from sharp from explicit calculation of Ψ^N, see Proposition C.3. We briefly discuss a possible route to a tighter bound in Remark C.2, but do not otherwise pursue this approach in this work.

We now explain how to obtain error estimates over a large enough range of α values to prove $v(\alpha)$ has a zero. We seek a solution of $H^\alpha \psi^\alpha = 0$ in $L^2_{K,1,1}$ with the form

$$\psi^\alpha(\boldsymbol{r}) = \psi^{N,\alpha}(\boldsymbol{r}) + \eta^\alpha(\boldsymbol{r}), \quad \psi^{N,\alpha}(\boldsymbol{r}) := \sum_{n=0}^{N} \alpha^n \Psi^n(\boldsymbol{r}). \tag{IV.5}$$

For arbitrary α, let Q^α denote the projection in $L^2_{K,1}$ onto $\psi^{N,\alpha}(\boldsymbol{r})$, and $Q^{\alpha,\perp} := I - Q^\alpha$ (note that $Q^0 = P$). Note that Q^α depends on N but we suppress this to avoid clutter. We assume WLOG that $Q^\alpha \eta^\alpha(\boldsymbol{r}) = 0$. It follows that η^α satisfies

$$Q^{\alpha,\perp} H^\alpha Q^{\alpha,\perp} \eta^\alpha = -\alpha^{N+1} Q^{\alpha,\perp} H^1 \Psi^N.$$

To obtain a bound on η^α in $L^2(\Omega)$, we require a lower bound on the operator $Q^{\alpha,\perp} H^\alpha Q^{\alpha,\perp} : Q^{\alpha,\perp} L^2_{K,1} \to Q^{\alpha,\perp} L^2_{K,1}$. The following Lemma gives a lower bound on this operator in terms of a lower bound on the projection of this operator onto the finite dimensional subspace of $L^2_{K,1}$ corresponding to a finite subset of the eigenfunctions of H^0. The importance of this result is that, since H^1 only couples finitely many modes of H^0, for *fixed* N, by taking the subset sufficiently large, we can always arrange that $\psi^{N,\alpha}(\boldsymbol{r})$ lies in this subspace.

Lemma IV.1. *Let P_Ξ denote the projection onto a subset Ξ of the eigenfunctions of H^0 in $L^2_{K,1}$, and let $\mu \geq 0$ be maximal such that*

$$\| P_\Xi^\perp H^0 P_\Xi^\perp \| \geq \mu, \quad P_\Xi^\perp := I - P_\Xi \tag{IV.6}$$

(with this notation the operator P introduced in Proposition IV.1 corresponds to P_Ξ with Ξ being the set $\{e_1(\boldsymbol{r})\}$ and $\mu = 1$). Suppose that $Q^\alpha P_\Xi = P_\Xi Q^\alpha = Q^\alpha$, i.e., that $\psi^{N,\alpha}(\boldsymbol{r})$ lies in $\operatorname{ran} P_\Xi$. *Define g^α by*

$$g^\alpha := \min \left\{ |E| : \begin{array}{l} E \textit{ is an eigenvalue of the matrix } Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp} \\ \textit{acting } Q^{\alpha,\perp} P_\Xi L^2_{K,1} \to Q^{\alpha,\perp} P_\Xi L^2_{K,1} \end{array} \right\}.$$

We note that $P_\Xi Q^{\alpha,\perp}$ is the projection onto the subspace of $P_\Xi L^2_{K,1}$ orthogonal to $\psi^{N,\alpha}(\boldsymbol{r})$. As long as

$$3\alpha \leq \mu \textit{ and } \alpha \| Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp \| < \min(g^\alpha, \mu - 3\alpha),$$

then

$$\| Q^{\alpha,\perp} H^\alpha Q^{\alpha,\perp} \eta^\alpha \| \geq \left(\min(g^\alpha, \mu - 3\alpha) - \alpha \| Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp \| \right) \| Q^{\alpha,\perp} \eta^\alpha \|. \tag{IV.7}$$

Note that g^α would be identically zero if not for the restriction that the matrix acts on $Q^{\alpha,\perp} P_\Xi L^2_{K,1}$, since otherwise $\psi^{N,\alpha}(\boldsymbol{r})$ would be an eigenfunction with eigenvalue zero for all α. As it is, $g^0 = 1$ and $\alpha \mapsto g^\alpha$ is analytic so that g^α must be positive for a non-zero interval of positive α values.

Proof. Using $Q^\alpha P_\Xi = P_\Xi Q^\alpha$ we have $P_\Xi^\perp Q^{\alpha,\perp} = Q^{\alpha,\perp} P_\Xi^\perp = P_\Xi^\perp$ and hence

$$\begin{aligned}&\|Q^{\alpha,\perp} H^\alpha Q^{\alpha,\perp}\eta^\alpha\| = \|Q^{\alpha,\perp}(P_\Xi + P_\Xi^\perp) H^\alpha (P_\Xi + P_\Xi^\perp) Q^{\alpha,\perp}\eta^\alpha\|\\ &= \|Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha + \alpha Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp \eta^\alpha + \alpha P_\Xi^\perp H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha + P_\Xi^\perp H^\alpha P_\Xi^\perp \eta^\alpha\|.\end{aligned}$$

By the reverse triangle inequality

$$\begin{aligned}&\|Q^{\alpha,\perp} H^\alpha Q^{\alpha,\perp}\eta^\alpha\| \\ &\geq \left|\|Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha + P_\Xi^\perp H^\alpha P_\Xi^\perp \eta^\alpha\| - \alpha\|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp \eta^\alpha + P_\Xi^\perp H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha\|\right|.\end{aligned} \tag{IV.8}$$

We want to bound the second term above and the first term below. We start with the second term

$$\begin{aligned}&\|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp \eta^\alpha + P_\Xi^\perp H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha\|^2\\ &= \|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp \eta^\alpha\|^2 + \|P_\Xi^\perp H^1 P_\Xi Q^{\alpha,\perp}\eta^\alpha\|^2\\ &\leq \|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp\|^2 \left(\|P_\Xi^\perp \eta^\alpha\|^2 + \|P_\Xi Q^{\alpha,\perp}\eta^\alpha\|^2\right)\\ &= \|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp\|^2 \|Q^{\alpha,\perp}\eta^\alpha\|^2,\end{aligned}$$

where we use Pythagoras' theorem, $P_\Xi^\perp H^1 P_\Xi Q^{\alpha,\perp}\eta^\alpha = P_\Xi^\perp H^1 P_\Xi Q^{\alpha,\perp} P_\Xi Q^{\alpha,\perp}\eta^\alpha$ since $P_\Xi Q^{\alpha,\perp}$ is a projection, and $\|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp\| = \|P_\Xi^\perp H^1 P_\Xi Q^{\alpha,\perp}\|$. Hence we can bound

$$\|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp \eta^\alpha + P_\Xi^\perp H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha\| \leq \|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp\| \|Q^{\alpha,\perp}\eta^\alpha\|. \tag{IV.9}$$

For the first term, first note that using Proposition IV.2 and the spectral theorem

$$\begin{aligned}\|Q^{\alpha,\perp} P_\Xi^\perp H^\alpha P_\Xi^\perp Q^{\alpha,\perp}\eta^\alpha\| &\geq |\|Q^{\alpha,\perp} P_\Xi^\perp H^0 P_\Xi^\perp Q^{\alpha,\perp}\eta^\alpha\| - \alpha\|Q^{\alpha,\perp} P_\Xi^\perp H^1 P_\Xi^\perp Q^{\alpha,\perp}\eta^\alpha\||\\ &\geq (\mu - 3\alpha)\|P_\Xi^\perp Q^{\alpha,\perp}\eta^\alpha\|\end{aligned}$$

as long as $\mu \geq 3\alpha$. We now estimate

$$\begin{aligned}&\|Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha + P_\Xi^\perp H^\alpha P_\Xi^\perp \eta^\alpha\|^2\\ &= \|Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha\|^2 + \|P_\Xi^\perp H^\alpha P_\Xi^\perp \eta^\alpha\|^2\\ &\geq (g^\alpha)^2 \|Q^{\alpha,\perp} P_\Xi \eta^\alpha\|^2 + (\mu - 3\alpha)^2 \|P_\Xi^\perp \eta^\alpha\|^2\\ &\geq \min\left((g^\alpha)^2, (\mu - 3\alpha)^2\right)\left(\|Q^{\alpha,\perp} P_\Xi \eta^\alpha\|^2 + \|P_\Xi^\perp \eta^\alpha\|^2\right)\\ &= \min\left((g^\alpha)^2, (\mu - 3\alpha)^2\right)\|Q^{\alpha,\perp}\eta^\alpha\|^2.\end{aligned}$$

It follows that as long as $3\alpha \leq \mu$,

$$\|Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}\eta^\alpha + P_\Xi^\perp H^\alpha P_\Xi^\perp \eta^\alpha\| \geq \min(g^\alpha, \mu - 3\alpha)\|Q^{\alpha,\perp}\eta^\alpha\|. \tag{IV.10}$$

The conclusion now holds as long as $3\alpha \leq \mu$ and $\alpha\|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp\| \leq \min(g^\alpha, \mu - 3\alpha)$ upon substituting (IV.9) and (IV.10) into (IV.8). □

For Lemma IV.1 to be useful, we must check that it is possible to choose Ξ so that the bound (IV.7) is non-trivial, i.e., so that the constant is positive. We will prove the following in Appendix D.

Proposition IV.3. *There exists a subset Ξ of the eigenfunctions of H^0 such that*

1. *The maximal μ such that* (IV.6) *holds is $\mu = 7$.*

2. *$\psi^{8,\alpha}(\boldsymbol{r})$ defined by* (IV.5) *lies in* $\operatorname{ran} P_\Xi$.

3. *$\|P_\Xi H^1 P_\Xi^\perp\| = 1$ and hence $\|Q^{\alpha,\perp} P_\Xi H^1 P_\Xi^\perp\| \leq 1$.*

The set Ξ constructed in Proposition IV.3 is the set of $L^2_{K,1}$-eigenfunctions of H^0 with eigenvalues with magnitude $\leq 4\sqrt{3}$, augmented with two extra basis functions to ensure that $\|P_\Xi H^1 P_\Xi^\perp\| = 1$. Including all $L^2_{K,1}$-eigenfunctions of H^0 with eigenvalue magnitudes up to and including $4\sqrt{3}$ ensures that $\psi^{8,\alpha}(\boldsymbol{r})$ lies in $\operatorname{ran} P_\Xi$.

We require the following, which we discuss further, and check numerically, in Section E. In particular, we show that this assumption is equivalent to a bound below on the lowest eigenvalue of a positive semi-definite, Hermitian, 81×81 matrix.

Assumption IV.1. *Let Ξ be as in Proposition IV.3. Then for all $0 \leq \alpha \leq \frac{7}{10}$, we have $g^\alpha \geq \frac{3}{4}$.*

Assuming Proposition IV.3 and Assumption IV.1, the bound (IV.7) becomes, for all $0 \leq \alpha \leq \frac{7}{10}$,

$$\|Q^{\alpha,\perp} H^\alpha Q^{\alpha,\perp} \eta^\alpha\| \geq \left(\frac{3}{4} - \alpha \right) \|Q^{\alpha,\perp} \eta^\alpha\|.$$

We now assume the following, proved in Appendix C.

Proposition IV.4. $\|H^1 \Psi^8\| \leq \frac{3}{20}$.

We can now give the proof of Theorem IV.1.

Proof of Theorem IV.1. The proof follows immediately from Lemma IV.1, Proposition IV.3, Assumption IV.1, and Proposition IV.4. □

Appendix A: Derivation of expression for Fermi velocity in terms of $L^2_{K,1,1}$ zero mode of H^α

The Bloch eigenvalue problem for the TKV Hamiltonian at quasi-momentum $\boldsymbol{k}$ is

$$H^\alpha \psi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}) = E_{\boldsymbol{k}} \psi^\alpha_{\boldsymbol{k}}(\boldsymbol{r})$$

where H^α is as in (II.1) and

$$\psi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{v}) = e^{i\boldsymbol{k}\cdot\boldsymbol{v}} \operatorname{diag}(1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}, 1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}) \psi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}) \quad \forall \boldsymbol{v} \in \Lambda.$$

By Propositions III.5 and III.6, 0 is a two-fold (at least) degenerate eigenvalue at the moiré K point $\boldsymbol{k} = 0$, with associated eigenfunctions $\psi^\alpha_{\pm 1}(\boldsymbol{r})$ as in Proposition III.6. In what follows we assume that 0 is *exactly* two-fold degenerate so that $\psi^\alpha_{\pm 1}(\boldsymbol{r})$ form a basis of the degenerate eigenspace. This assumption is clearly true for small α but could in principle be violated for $\alpha > 0$.

Introducing $\chi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}) := e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \psi^\alpha_{\boldsymbol{k}}(\boldsymbol{r})$, we derive the equivalent Bloch eigenvalue problem with $\boldsymbol{k}$-independent boundary conditions

$$H^\alpha_{\boldsymbol{k}} \chi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}) = E_{\boldsymbol{k}} \chi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}), \tag{A.1}$$

where

$$H^\alpha_{\boldsymbol{k}} := \begin{pmatrix} 0 & D^{\alpha\dagger}_{\boldsymbol{k}} \\ D^\alpha_{\boldsymbol{k}} & 0 \end{pmatrix}, \quad D^\alpha_{\boldsymbol{k}} = \begin{pmatrix} D_x + k_x + i(D_y + k_y) & \alpha U(\boldsymbol{r}) \\ \alpha U(-\boldsymbol{r}) & D_x + k_x + i(D_y + k_y) \end{pmatrix},$$

where $D_{x,y} := -i\partial_{x,y}$, and

$$\chi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{v}) = \operatorname{diag}(1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}, 1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}) \chi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}) \quad \forall \boldsymbol{v} \in \Lambda.$$

Clearly $\psi^\alpha_{\pm 1}(\boldsymbol{r})$ remain a basis of the zero eigenspace for the problem (A.1) at $\boldsymbol{k} = 0$.

Differentiating the operator $D^\alpha_{\boldsymbol{k}}$ we find $\partial_{k_x} D^\alpha_{\boldsymbol{k}} = I_2$ and $\partial_{k_y} D^\alpha_{\boldsymbol{k}} = iI_2$, where I_2 denotes the 2×2 identity matrix, so that

$$\partial_{k_x} H^\alpha_{\boldsymbol{k}} = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}, \quad \partial_{k_y} H^\alpha_{\boldsymbol{k}} = \begin{pmatrix} 0 & -iI_2 \\ iI_2 & 0 \end{pmatrix}. \tag{A.2}$$

By degenerate perturbation theory[9], for small $\boldsymbol{k}$ we have that eigenfunctions $\chi^\alpha_{\boldsymbol{k}}(\boldsymbol{r})$ of (A.1) are given by

$$\chi^\alpha_{\boldsymbol{k}}(\boldsymbol{r}) \approx \sum_{\sigma = \pm 1} c_{\sigma,\boldsymbol{k}} \psi^\alpha_\sigma(\boldsymbol{r}),$$

where the coefficients $c_{\sigma,\boldsymbol{k}}$ and associated eigenvalues $E_{\boldsymbol{k}} \approx \epsilon_{\boldsymbol{k}}$ are found by solving the matrix eigenvalue problem

$$\begin{pmatrix} \frac{\langle \psi_1^\alpha | \boldsymbol{k}\cdot\nabla_{\boldsymbol{k}} H_{\boldsymbol{0}}^\alpha \psi_1^\alpha \rangle}{\langle \psi_1^\alpha | \psi_1^\alpha \rangle} & \frac{\langle \psi_1^\alpha | \boldsymbol{k}\cdot\nabla_{\boldsymbol{k}} H_{\boldsymbol{0}}^\alpha \psi_{-1}^\alpha \rangle}{\langle \psi_1^\alpha | \psi_1^\alpha \rangle} \\ \frac{\langle \psi_{-1}^\alpha | \boldsymbol{k}\cdot\nabla_{\boldsymbol{k}} H_{\boldsymbol{0}}^\alpha \psi_1^\alpha \rangle}{\langle \psi_{-1}^\alpha | \psi_{-1}^\alpha \rangle} & \frac{\langle \psi_{-1}^\alpha | \boldsymbol{k}\cdot\nabla_{\boldsymbol{k}} H_{\boldsymbol{0}}^\alpha \psi_{-1}^\alpha \rangle}{\langle \psi_{-1}^\alpha | \psi_{-1}^\alpha \rangle} \end{pmatrix} \begin{pmatrix} c_{+1,\boldsymbol{k}} \\ c_{-1,\boldsymbol{k}} \end{pmatrix} = \epsilon_{\boldsymbol{k}} \begin{pmatrix} c_{+1,\boldsymbol{k}} \\ c_{-1,\boldsymbol{k}} \end{pmatrix}. \tag{A.3}$$

Using (A.2) and the explicit forms of $\psi_{\pm 1}^\alpha(\boldsymbol{r})$ given by Proposition III.6, we find that the matrix on the left-hand side of (A.3) can be simplified to

$$\begin{pmatrix} 0 & \lambda(\alpha)(k_x - ik_y) \\ \lambda^*(\alpha)(k_x + ik_y) & 0 \end{pmatrix}, \quad \lambda(\alpha) := \frac{\langle \psi_1^\alpha(\boldsymbol{r}) | \, \psi_1^{\alpha *}(-\boldsymbol{r}) \rangle}{\langle \psi_1^\alpha(\boldsymbol{r}) | \, \psi_1^\alpha(\boldsymbol{r}) \rangle}.$$

It follows that, for small $\boldsymbol{k}$, we have $E_{\boldsymbol{k}} \approx \pm v(\alpha)|\boldsymbol{k}|$, where $v(\alpha) = |\lambda(\alpha)|$ is as in (III.8).

Appendix B: The chiral basis of $L^2_{K,1}$ and action of H^0 and H^1 with respect to this basis

1. The spectrum and eigenfunctions of H^0 in L^2_K

The first task is to understand the spectrum and eigenfunctions of H^0 in L^2_K. In the next section we will discuss the spectrum and eigenfunctions of H^0 in $L^2_{K,1}$. Recall that

$$H^0 = \begin{pmatrix} 0 & D^{0\dagger} \\ D^0 & 0 \end{pmatrix}, \quad D^0 = \begin{pmatrix} -2i\overline{\partial} & 0 \\ 0 & -2i\overline{\partial} \end{pmatrix},$$

where $\overline{\partial} = \frac{1}{2}(\partial_x + i\partial_y)$. To describe the eigenfunctions of H^0 in L^2_K we introduce some notation. Let $\boldsymbol{v} = \left(v_1, v_2\right)$ be a vector in $\mathbb{R}^2$. Then we will write

$$z_{\boldsymbol{v}} = v_1 + iv_2, \quad \hat{z}_{\boldsymbol{v}} = \frac{v_1 + iv_2}{|\boldsymbol{v}|}.$$

Finally, let V denote the area of the moiré cell Ω.

Proposition B.1. *The zero eigenspace of H^0 in L^2_K is spanned by*

$$\chi_\pm^{\boldsymbol{0}}(\boldsymbol{r}) = \frac{1}{\sqrt{2V}} \left(1, 0, \pm 1, 0\right).$$

For all $\boldsymbol{G} \neq 0$ in the reciprocal lattice, then

$$\chi_\pm^{\boldsymbol{G}}(\boldsymbol{r}) = \frac{1}{\sqrt{2V}} \left(1, 0, \pm \hat{z}_{\boldsymbol{G}}, 0\right) e^{i\boldsymbol{G}\cdot\boldsymbol{r}}$$

are eigenfunctions with eigenvalues $\pm|\boldsymbol{G}|$*. For all* $\boldsymbol{G}$ *in the reciprocal lattice,*

$$\chi_{\pm}^{\boldsymbol{q}_1+\boldsymbol{G}}(\boldsymbol{r}) = \frac{1}{\sqrt{2V}}\left(0, 1, 0, \pm\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1}\right) e^{i(\boldsymbol{q}_1+\boldsymbol{G})\cdot\boldsymbol{r}}$$

are eigenfunctions with eigenvalues $\pm|\boldsymbol{q}_1+\boldsymbol{G}|$*. The operator* H^0 *has no other eigenfunctions in* L^2_K *other than linear combinations of these, and hence the spectrum of* H^0 *in* L^2_K *is*

$$\sigma_{L^2_K}(H^0) = \{\pm|\boldsymbol{G}|, \pm|\boldsymbol{q}_1+\boldsymbol{G}| : \boldsymbol{G} \in \Lambda^*\}.$$

Proof. The proof is a straightforward calculation taking into account the L^2_K boundary conditions given by (III.6) with $\boldsymbol{k} = 0$. For example, $e_2(\boldsymbol{r})$ and $e_4(\boldsymbol{r})$ are zero eigenfunctions of H^0 but in $L^2_{K'}$, not L^2_K. □

Note that (as it must be because of the chiral symmetry) the spectrum is symmetric about 0 and all of the eigenfunctions with negative eigenvalues are given by applying $\mathcal{S}$ to the eigenfunctions with positive eigenvalues.

The union of the lattices Λ^* and $\Lambda^*+\boldsymbol{q}_1$ has the form of a honeycomb lattice in momentum space, where the lattice Λ^* corresponds to "A" sites and $\Lambda^*+\boldsymbol{q}_1$ corresponds to "B" sites (or vice versa), see Figure B.1.

2. The spectrum and eigenfunctions of H^0 in $L^2_{K,1}$

We now discuss the spectrum of H^0 in $L^2_{K,1}$.

Proposition B.2. *The zero eigenspace of* H^0 *in* $L^2_{K,1}$ *is spanned by*

$$\chi^{\widetilde{\boldsymbol{0}}}(\boldsymbol{r}) := \frac{1}{\sqrt{V}} e_1(\boldsymbol{r}).$$

For all $\boldsymbol{G} \neq 0$ *in the reciprocal lattice* Λ^**,*

$$\chi_{\pm}^{\widetilde{\boldsymbol{G}}}(\boldsymbol{r}) := \frac{1}{\sqrt{3}}\sum_{k=0}^{2}\mathcal{R}^k\chi_{\pm}^{\boldsymbol{G}}(\boldsymbol{r}) = \frac{1}{\sqrt{3}}\sum_{k=0}^{2}\chi_{\pm}^{(R_\phi^*)^k\boldsymbol{G}}(\boldsymbol{r})$$

are eigenfunctions of H^0 *in* $L^2_{K,1}$ *with associated eigenvalues* $\pm|\boldsymbol{G}|$*. For all* $\boldsymbol{G}$ *in the reciprocal lattice* Λ^**,*

$$\chi^{\pm\widetilde{\boldsymbol{G}+\boldsymbol{q}_1}}(\boldsymbol{r}) = \frac{1}{\sqrt{3}}\sum_{k=0}^{2}\mathcal{R}^k\chi_{\pm}^{\boldsymbol{G}+\boldsymbol{q}_1}(\boldsymbol{r}) = \frac{1}{\sqrt{3}}\sum_{k=0}^{2}\chi_{\pm}^{(R_\phi^*)^k(\boldsymbol{G}+\boldsymbol{q}_1)}(\boldsymbol{r})$$

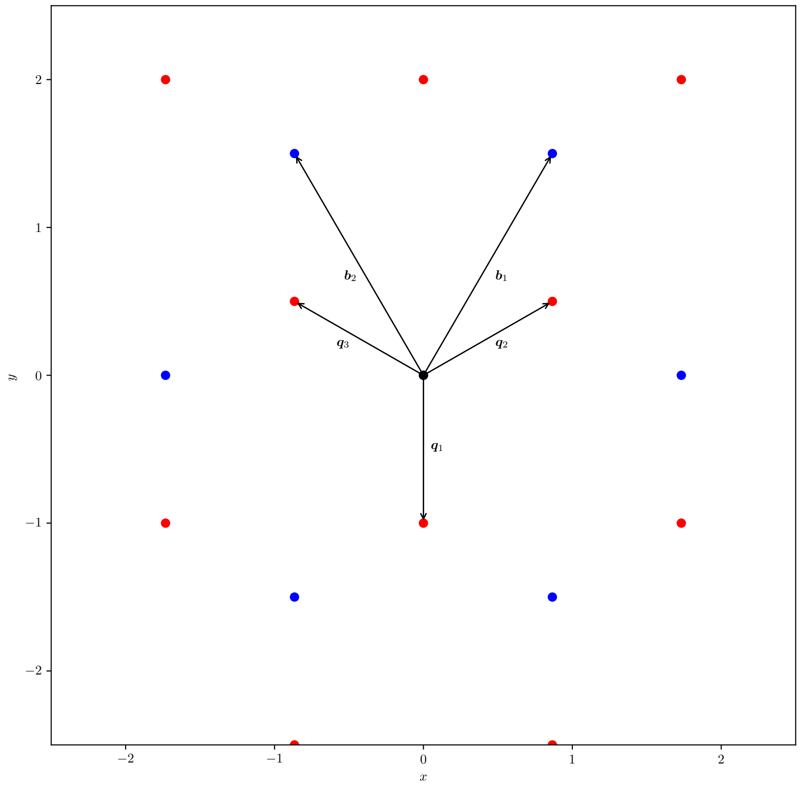

FIG. B.1. Diagram showing A (blue) and B (red) sites of the momentum space lattice. Each site corresponds to two L^2_K-eigenvalues of H^0, given by $\pm$ the distance between the site and the origin (black). The lattice vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ are shown, as well as the A site nearest-neighbor vectors $\boldsymbol{q}_1$, $\boldsymbol{q}_2$, $\boldsymbol{q}_3$.

are eigenfunctions of H^0 *in* $L^2_{K,1}$ *with associated eigenvalues* $\pm|\boldsymbol{q}_1 + \boldsymbol{G}|$. *The operator* H^0 *has no other eigenfunctions in* $L^2_{K,1}$ *other than linear combinations of these, and hence the spectrum of* H^0 *in* $L^2_{K,1}$ *is*

$$\sigma_{L^2_{K,1}}(H^0) = \{\pm|\boldsymbol{G}|, \pm|\boldsymbol{q}_1 + \boldsymbol{G}| : \boldsymbol{G} \in \Lambda^*\}\,.$$

Proof. The proof is another straightforward calculation starting from Proposition B.1. □

For an illustration of the support of the $L^2_{K,1}$-eigenfunctions of H^0 on the momentum space lattice, see Figure B.2. It is important to note that the notation introduced in Proposition

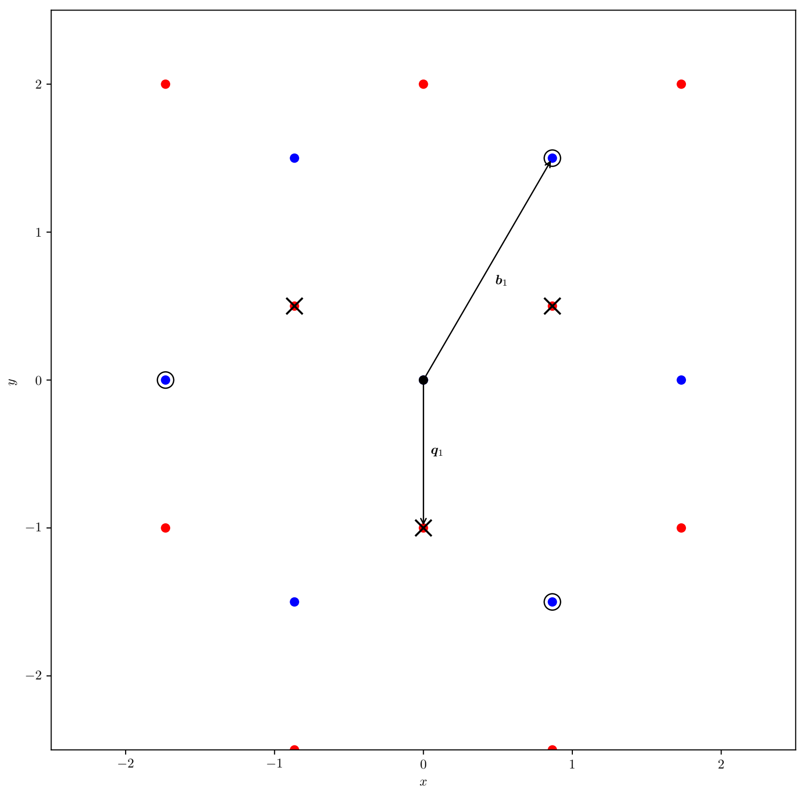

FIG. B.2. Diagram showing support of $L^2_{K,1}$-eigenfunctions of H^0 superposed on the momentum space lattice. Each eigenfunction is given by superposing an L^2_K-eigenfunction of H^0 with its rotations by $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$. The support of the eigenfunctions $\chi^{\pm\widetilde{\boldsymbol{q}_1}}(\boldsymbol{r})$ with eigenvalues ± 1 is shown with black crosses, while the support of the eigenfunctions $\chi^{\pm\widetilde{\boldsymbol{b}_1}}(\boldsymbol{r})$ with eigenvalues $\pm\sqrt{3}$ is shown with black circles.

B.2 is not one-to-one, because for example

$$\chi^{\pm\widetilde{\boldsymbol{G}}}(\boldsymbol{r}) = \chi^{\pm\widetilde{R^*_\phi \boldsymbol{G}}}(\boldsymbol{r}) = \chi^{\pm\widetilde{(R^*_\phi)^2 \boldsymbol{G}}}(\boldsymbol{r})$$

for any $\boldsymbol{G} \neq 0$ in Λ^*.

3. The chiral basis of $L^2_{K,1}$

Recall that zero modes of H^α can be assumed to be eigenfunctions of the chiral symmetry operator $\mathcal{S}$. It follows that the most convenient basis for our purposes is not be the spectral basis just introduced but the basis of $L^2_{K,1}$ consisting of eigenfunctions of $\mathcal{S}$. We call this basis the chiral basis.

Definition B.1. *The chiral basis of $L^2_{K,1}$ is defined as the union of the functions*

$$\chi^{\widetilde{\mathbf{0}}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} e_1,$$

$$\chi^{\widetilde{\boldsymbol{G}},\pm 1}(\boldsymbol{r}) := \frac{1}{\sqrt{2}} \left(\chi^{\widetilde{\boldsymbol{G}}}(\boldsymbol{r}) \pm \chi^{-\widetilde{\boldsymbol{G}}}(\boldsymbol{r}) \right), \quad \boldsymbol{G} \in \Lambda^* \setminus \{\mathbf{0}\},$$

and

$$\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{G}},\pm 1}(\boldsymbol{r}) := \frac{1}{\sqrt{2}} \left(\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{G}}}(\boldsymbol{r}) \pm \chi^{-\widetilde{\boldsymbol{q}_1+\boldsymbol{G}}}(\boldsymbol{r}) \right), \quad \boldsymbol{G} \in \Lambda^*.$$

The following is straightforward.

Proposition B.3. *The chiral basis is an orthonormal basis of $L^2_{K,1}$. The modes $\chi^{\widetilde{\mathbf{0}}}(\boldsymbol{r})$, $\chi^{\widetilde{\boldsymbol{G}},1}(\boldsymbol{r})$, and $\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{G}},1}(\boldsymbol{r})$ are $+1$ eigenfunctions of $\mathcal{S}$, while the modes $\chi^{\widetilde{\boldsymbol{G}},-1}(\boldsymbol{r})$ and $\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{G}},-1}(\boldsymbol{r})$ are -1 eigenfunctions of $\mathcal{S}$.*

Written out, chiral basis functions have a very simple form. We have

$$\chi^{\widetilde{\mathbf{0}}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} e_1, \tag{B.1}$$

and for all $\boldsymbol{G} \in \Lambda^* \setminus \{\mathbf{0}\}$,

$$\chi^{\widetilde{\boldsymbol{G}},1}(\boldsymbol{r}) = \frac{1}{\sqrt{3V}} e_1 \sum_{k=0}^{2} e^{i((R_\phi^*)^k \boldsymbol{G}) \cdot \boldsymbol{r}}, \quad \chi^{\widetilde{\boldsymbol{G}},-1}(\boldsymbol{r}) = \frac{1}{\sqrt{3V}} \hat{z}_{\boldsymbol{G}} e_3 \sum_{k=0}^{2} e^{-ik\phi} e^{i((R_\phi^*)^k \boldsymbol{G}) \cdot \boldsymbol{r}}, \tag{B.2}$$

and for all $\boldsymbol{G} \in \Lambda^*$,

$$\begin{aligned} \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1},1}(\boldsymbol{r}) &= \frac{1}{\sqrt{3V}} e_2 \sum_{k=0}^{2} e^{i((R_\phi^*)^k (\boldsymbol{q}_1 + \boldsymbol{G})) \cdot \boldsymbol{r}}, \\ \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1},-1}(\boldsymbol{r}) &= \frac{1}{\sqrt{3V}} \hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1} e_4 \sum_{k=0}^{2} e^{-ik\phi} e^{i((R_\phi^*)^k (\boldsymbol{q}_1 + \boldsymbol{G})) \cdot \boldsymbol{r}}. \end{aligned} \tag{B.3}$$

We use the chiral basis to divide up $L^2_{K,1}$ as follows.

Definition B.2. *We define spaces $L^2_{K,1,\pm 1}$ to be the spans of the ± 1 eigenfunctions of $\mathcal{S}$ in $L^2_{K,1}$, respectively.*

Clearly we have

$$L^2_{K,1} = L^2_{K,1,1} \oplus L^2_{K,1,-1}.$$

We can divide up the chiral basis more finely as follows.

Definition B.3. *We define*

$$
\begin{aligned}
L^2_{K,1,1,A} &:= \left\{ \chi^{\widetilde{\mathbf{0}}}(\boldsymbol{r}) \right\} \cup \left\{ \chi^{\widetilde{\boldsymbol{G}},1}(\boldsymbol{r}) : \boldsymbol{G} \in \Lambda^* \setminus \{\mathbf{0}\} \right\}, \\
L^2_{K,1,1,B} &:= \left\{ \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1},1}(\boldsymbol{r}) : \boldsymbol{G} \in \Lambda^* \right\}, \\
L^2_{K,1,-1,A} &:= \left\{ \chi^{\widetilde{\boldsymbol{G}},-1}(\boldsymbol{r}) : \boldsymbol{G} \in \Lambda^* \setminus \{\mathbf{0}\} \right\}, \\
L^2_{K,1,-1,B} &:= \left\{ \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1},-1}(\boldsymbol{r}) : \boldsymbol{G} \in \Lambda^* \right\}.
\end{aligned}
$$

Remark B.1. *Note that the notation A and B in Definition B.3 refers to A and B sites of the momentum space lattice, not to the A and B sites of the real space lattice. Recalling Remark III.1 and comparing* (B.2)-(B.3) *with* (II.2)*, we see that $L^2_{K,1,1,A}$ corresponds to wave-functions supported on A sites of layer* 1*, $L^2_{K,1,1,B}$ corresponds to wave-functions supported on A sites of layer* 2*, $L^2_{K,1,-1,A}$ corresponds to wave-functions supported on B sites of layer* 1*, and $L^2_{K,1,-1,B}$ corresponds to wave-functions supported on B sites of layer* 2*.*

Clearly we have

$$
L^2_{K,1} = L^2_{K,1,1,A} \oplus L^2_{K,1,1,B} \oplus L^2_{K,1,-1,A} \oplus L^2_{K,1,-1,B}.
$$

The following propositions are straightforward to prove. For the first claim, note that $\{\mathcal{S}, H^0\} = 0$.

Proposition B.4. *The operator H^0 maps $L^2_{K,1,\pm1,\sigma} \to L^2_{K,1,\mp1,\sigma}$ for $\sigma = A, B$. The action of H^0 on chiral basis functions is as follows*

$$
H^0 \chi^{\widetilde{\mathbf{0}}} = 0,
$$

for all $\boldsymbol{G} \in \Lambda^*$ with $\boldsymbol{G} \neq 0$

$$
H^0 \chi^{\widetilde{\boldsymbol{G}},\pm1} = |\boldsymbol{G}| \chi^{\widetilde{\boldsymbol{G}},\mp1},
$$

and for all $\boldsymbol{G} \in \Lambda^*$

$$
H^0 \chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{G}},\pm1} = |\boldsymbol{q}_1 + \boldsymbol{G}| \chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{G}},\mp1}.
$$

Proposition B.5. *Let P denote the projection operator onto $\chi^{\widetilde{\mathbf{0}}}(\boldsymbol{r})$ in $L^2_{K,1}$, and $P^\perp = 1 - P$. Then the operator $P^\perp (H^0)^{-1} P^\perp$ maps $L^2_{K,1,\pm1,\sigma} \to L^2_{K,1,\mp1,\sigma}$ for $\sigma = A, B$, and*

$$
P^\perp (H^0)^{-1} P^\perp \chi^{\widetilde{\boldsymbol{G}},\pm1} = \frac{1}{|\boldsymbol{G}|} \chi^{\widetilde{\boldsymbol{G}},\mp1}
$$

for all $\boldsymbol{G} \in \Lambda^*$ *with* $\boldsymbol{G} \neq 0$*, and*

$$P^{\perp}(H^0)^{-1}P^{\perp}\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{G}},\pm 1} = \frac{1}{|\boldsymbol{q}_1+\boldsymbol{G}|}\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{G}},\mp 1}$$

for all $\boldsymbol{G} \in \Lambda^*$.

In the coming sections we will study the action of the operator H^1 on $L^2_{K,1}$ with respect to the chiral basis.

4. The spectrum of H^1 in L^2_K and $L^2_{K,1}$

Recall that

$$H^1 = \begin{pmatrix} 0 & D^{1\dagger} \\ D^1 & 0 \end{pmatrix}, \quad D^1 = \begin{pmatrix} 0 & U(\boldsymbol{r}) \\ U(-\boldsymbol{r}) & 0 \end{pmatrix},$$

where $U(\boldsymbol{r}) = e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{i\phi}e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}} + e^{-i\phi}e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}$. We claim the following.

Proposition B.6. *For each* $\boldsymbol{r}_0 \in \Omega$*,* $\pm|U(\boldsymbol{r}_0)|$ *and* $\pm|U(-\boldsymbol{r}_0)|$ *are eigenvalues of* $H^1 : L^2_K \to L^2_K$*. For* $\boldsymbol{r}_0$ *such that* $U(\boldsymbol{r}_0) \neq 0$*, the* $\pm|U(\boldsymbol{r}_0)|$ *eigenvectors are*

$$\left(0, 1, \pm\tfrac{U(\boldsymbol{r}_0)}{|U(\boldsymbol{r}_0)|}, 0\right)\delta(\boldsymbol{r}-\boldsymbol{r}_0).$$

For $\boldsymbol{r}_0$ *such that* $U(-\boldsymbol{r}_0) \neq 0$*, the* $\pm|U(-\boldsymbol{r}_0)|$ *eigenvectors are*

$$\left(1, 0, 0, \pm\tfrac{U(-\boldsymbol{r}_0)}{|U(-\boldsymbol{r}_0)|}\right)\delta(\boldsymbol{r}-\boldsymbol{r}_0).$$

When $U(\boldsymbol{r}_0) = 0$*, zero is a degenerate eigenvalue with associated eigenfunctions* $e_2\delta(\boldsymbol{r}-\boldsymbol{r}_0)$ *and* $e_3\delta(\boldsymbol{r}-\boldsymbol{r}_0)$*. When* $U(-\boldsymbol{r}_0) = 0$*, zero is a degenerate eigenvalue with associated eigenfunctions* $e_1\delta(\boldsymbol{r}-\boldsymbol{r}_0)$ *and* $e_4\delta(\boldsymbol{r}-\boldsymbol{r}_0)$*. Finally,*

$$\sigma_{L^2_K}(H^1) = [-3, 3]. \tag{B.4}$$

Proof. We prove only (B.4) since the other assertions are clear. The triangle inequality yields the obvious bound

$$|U(\boldsymbol{r}_0)| \leq 3,$$

so that the L^2_K spectrum of H^1 must be contained in the interval $[-3, 3]$. To see that the spectrum actually equals $[-3, 3]$, note that if $\boldsymbol{r}_0 = \left(\frac{4\pi}{3\sqrt{3}}, 0\right)$ then

$$\boldsymbol{q}_1\cdot\boldsymbol{r}_0 = 0, (\boldsymbol{q}_1+\boldsymbol{b}_1)\cdot\boldsymbol{r}_0 = \frac{1}{2}\left(\sqrt{3}, 1\right)\cdot\boldsymbol{r}_0 = \frac{2\pi}{3}, (\boldsymbol{q}_1+\boldsymbol{b}_2)\cdot\boldsymbol{r}_0 = \frac{1}{2}\left(-\sqrt{3}, 1\right)\cdot\boldsymbol{r}_0 = -\frac{2\pi}{3}$$

and hence $U(\boldsymbol{r}_0) = 3$. On the other hand, when $\boldsymbol{r}_0 = 0$ we have $U(\boldsymbol{r}_0) = 0$ so that the spectrum of H^1 in L^2_K equals $[-3, 3]$. □

By taking linear combinations of rotated copies of the H^1 eigenfunctions, just as we did with the H^0 eigenfunctions, it is straightforward to prove an analogous result to Proposition B.6 in $L^2_{K,1}$. We record only the following.

Proposition B.7.

$$\sigma_{L^2_{K,1}}(H^1) = [-3, 3].$$

5. The action of H^1 on $L^2_{K,1}$ with respect to the chiral basis

We now want to study the action of H^1 on $L^2_{K,1}$ with respect to the chiral basis. We will prove two propositions, which parallel Proposition B.4.

Proposition B.8. *The operator H^1 maps $L^2_{K,1,1,A} \to L^2_{K,1,-1,B}$, and $L^2_{K,1,1,B} \to L^2_{K,1,-1,A}$. The action of H^1 on chiral basis functions is as follows:*

$$H^1 \chi^{\widetilde{\boldsymbol{0}}} = \sqrt{3} \overline{\hat{z}_{\boldsymbol{q}_1}} \chi^{\widetilde{\boldsymbol{q}_1,-1}}, \tag{B.5}$$

and

$$H^1 \chi^{\widetilde{\boldsymbol{q}_1,1}} = e^{i\phi} \overline{\hat{z}_{\boldsymbol{q}_1 - \boldsymbol{q}_2}} \chi^{\widetilde{\boldsymbol{q}_1 - \boldsymbol{q}_2,-1}} + e^{-i\phi} \overline{\hat{z}_{\boldsymbol{q}_1 - \boldsymbol{q}_3}} \chi^{\widetilde{\boldsymbol{q}_1 - \boldsymbol{q}_3,-1}} \tag{B.6}$$

For all $\boldsymbol{G} \in \Lambda^* \setminus \{\boldsymbol{0}\}$,

$$H^1 \chi^{\widetilde{\boldsymbol{G},1}} = \overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1}} \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1,-1}} + e^{i\phi} \overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_2}} \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_2,-1}} + e^{-i\phi} \overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_3}} \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_3,-1}} \tag{B.7}$$

For all $\boldsymbol{G} \in \Lambda^* \setminus \{\boldsymbol{0}\}$,

$$H^1 \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1,1}} = \overline{\hat{z}_{\boldsymbol{G}}} \chi^{\widetilde{\boldsymbol{G},-1}} + e^{i\phi} \overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_2}} \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_2,-1}} + e^{-i\phi} \overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_3}} \chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_3,-1}}. \tag{B.8}$$

Note that H^1 exchanges chirality ($\mathcal{S}$ eigenvalue) and the A and B momentum space sublattices, while H^0 only exchanges chirality. Proposition B.8 has a simple interpretation in terms of nearest-neighbor hopping in the momentum space lattice, see Figures B.3 and B.4.

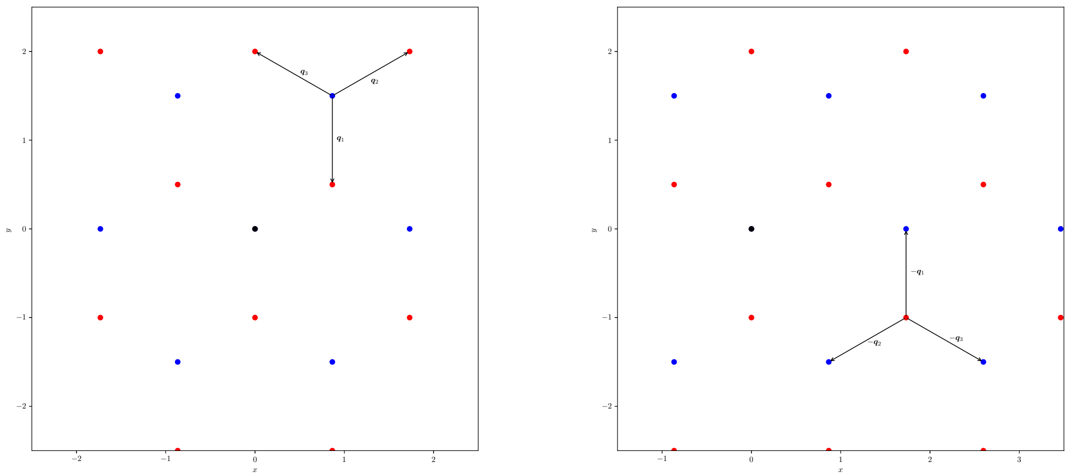

FIG. B.3. Illustration of the action of H^1 in $L^2_{K,1}$ as hopping in the momentum space lattice described by equations (B.7) (left, starting at $\boldsymbol{b}_1$) and (B.8) (right, starting at $\boldsymbol{q}_1 + \boldsymbol{b}_1 - \boldsymbol{b}_2$). The origin is marked by a black dot.

Remark B.2. *At first glance, equations* (B.5) *and* (B.6) *appear different from* (B.7) *and* (B.8)*, because they appear to violate* $\frac{2\pi}{3}$ *rotation symmetry. But this is not the case, since every chiral basis function individually respects this symmetry. For example, using* $\chi^{\widetilde{\boldsymbol{q}_1},-1} = \chi^{\widetilde{\boldsymbol{q}_2},-1} = \chi^{\widetilde{\boldsymbol{q}_3},-1}$ *and* $\overline{\hat{z}_{\boldsymbol{q}_1}} = e^{i\phi}\overline{\hat{z}_{\boldsymbol{q}_2}} = e^{-i\phi}\overline{\hat{z}_{\boldsymbol{q}_3}}$*, we can re-write* (B.5) *in a way that manifestly respects the* $\frac{2\pi}{3}$ *rotation symmetry as*

$$H^1\chi^{\widetilde{\boldsymbol{0}}} = \frac{1}{\sqrt{3}}\left(\overline{\hat{z}_{\boldsymbol{q}_1}}\chi^{\widetilde{\boldsymbol{q}_1},-1} + e^{i\phi}\overline{\hat{z}_{\boldsymbol{q}_2}}\chi^{\widetilde{\boldsymbol{q}_2},-1} + e^{-i\phi}\overline{\hat{z}_{\boldsymbol{q}_3}}\chi^{\widetilde{\boldsymbol{q}_3},-1}\right). \tag{B.9}$$

Equation (B.6) *can also be written in a manifestly rotationally invariant way but the expression is long and hence we omit it. Note that* (B.6) *cannot have a term proportional to* $\chi^{\widetilde{\boldsymbol{0}}}$ *since* $\chi^{\widetilde{\boldsymbol{0}}} \in L^2_{K,1,1}$ *and* H^1 *maps* $L^2_{K,1,1} \to L^2_{K,1,-1}$.

Proof of Proposition B.8. We will prove (B.7), the proofs of the other identities are similar and hence omitted. We have

$$H^1\chi^{\widetilde{\boldsymbol{G}},1} = \frac{1}{\sqrt{3V}}\left(e^{i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{i\phi}e^{i(\boldsymbol{q}_1+\boldsymbol{b}_1)\cdot\boldsymbol{r}} + e^{-i\phi}e^{i(\boldsymbol{q}_1+\boldsymbol{b}_2)\cdot\boldsymbol{r}}\right)\left(e^{i\boldsymbol{G}\cdot\boldsymbol{r}} + e^{i(R_\phi^*\boldsymbol{G})\cdot\boldsymbol{r}} + e^{i((R_\phi^*)^2\boldsymbol{G})\cdot\boldsymbol{r}}\right)e_4.$$

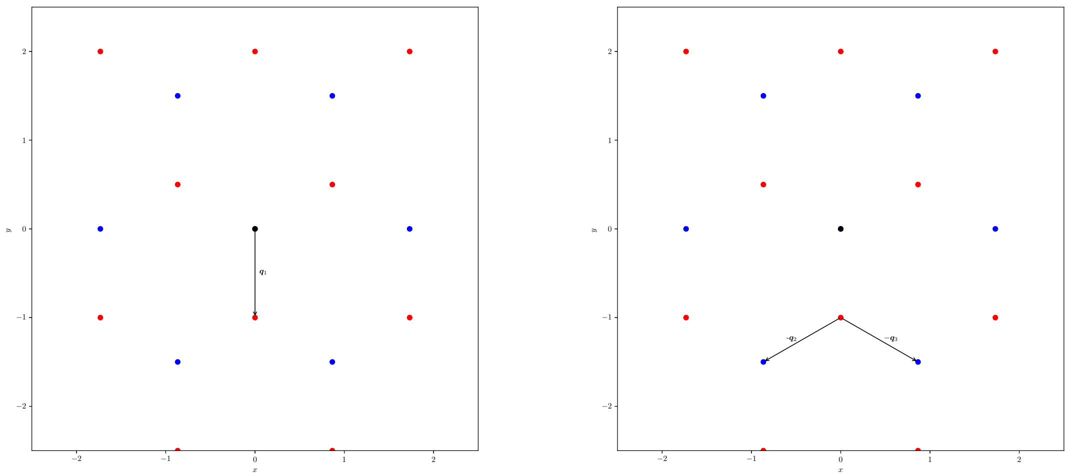

FIG. B.4. Illustration of the action of H^1 as hopping in the momentum space lattice described by equations (B.5) (left, starting at $\mathbf{0}$) and (B.6) (right, starting at $\boldsymbol{q}_1$). Although it appears that the hopping in these cases does not respect $\frac{2\pi}{3}$ rotation symmetry, this is an artifact of working with chiral basis functions which individually respect the rotation symmetry, see (B.9).

Multiplying out we have

$$
\begin{aligned}
&\frac{1}{\sqrt{3V}}\Big(e^{i(\boldsymbol{q}_1+\boldsymbol{G})\cdot\boldsymbol{r}}+e^{i\phi}e^{i(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_1)\cdot\boldsymbol{r}}+e^{-i\phi}e^{i(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_2)\cdot\boldsymbol{r}}\\
&+e^{i(\boldsymbol{q}_1+(R_\phi^*\boldsymbol{G}))\cdot\boldsymbol{r}}+e^{i\phi}e^{i(\boldsymbol{q}_1+(R_\phi^*\boldsymbol{G})+\boldsymbol{b}_1)\cdot\boldsymbol{r}}+e^{-i\phi}e^{i(\boldsymbol{q}_1+(R_\phi^*\boldsymbol{G})+\boldsymbol{b}_2)\cdot\boldsymbol{r}}\\
&+e^{i(\boldsymbol{q}_1+((R_\phi^*)^2\boldsymbol{G}))\cdot\boldsymbol{r}}+e^{i\phi}e^{i(\boldsymbol{q}_1+((R_\phi^*)^2\boldsymbol{G})+\boldsymbol{b}_1)\cdot\boldsymbol{r}}+e^{-i\phi}e^{i(\boldsymbol{q}_1+((R_\phi^*)^2\boldsymbol{G})+\boldsymbol{b}_2)\cdot\boldsymbol{r}}\Big)\\
=&\frac{1}{\sqrt{3V}}\Big(e^{i(\boldsymbol{q}_1+\boldsymbol{G})\cdot\boldsymbol{r}}+e^{i\phi}e^{i(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_1)\cdot\boldsymbol{r}}+e^{-i\phi}e^{i(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_2)\cdot\boldsymbol{r}}\\
&e^{i(R_\phi^*(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_1))\cdot\boldsymbol{r}}+e^{i\phi}e^{i(R_\phi^*(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_2))\cdot\boldsymbol{r}}+e^{-i\phi}e^{i(R_\phi^*(\boldsymbol{q}_1+\boldsymbol{G}))\cdot\boldsymbol{r}}\\
&+e^{i((R_\phi^*)^2(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_2))\cdot\boldsymbol{r}}+e^{i\phi}e^{i((R_\phi^*)^2(\boldsymbol{q}_1+\boldsymbol{G}))\cdot\boldsymbol{r}}+e^{-i\phi}e^{i((R_\phi^*)^2(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_1)\cdot\boldsymbol{r}}\Big).\\
=&\frac{1}{\sqrt{3V}}\left(e^{i(\boldsymbol{q}_1+\boldsymbol{G})\cdot\boldsymbol{r}}+e^{-i\phi}e^{i(R_\phi^*(\boldsymbol{q}_1+\boldsymbol{G}))\cdot\boldsymbol{r}}+e^{i\phi}e^{i((R_\phi^*)^2(\boldsymbol{q}_1+\boldsymbol{G}))\cdot\boldsymbol{r}}\right)\\
&+\frac{1}{\sqrt{3V}}e^{i\phi}\left(e^{i(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_1)\cdot\boldsymbol{r}}+e^{-i\phi}e^{i(R_\phi^*(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_1))\cdot\boldsymbol{r}}+e^{i\phi}e^{i((R_\phi^*)^2(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_1))\cdot\boldsymbol{r}}\right)\\
&+\frac{1}{\sqrt{3V}}e^{-i\phi}\left(e^{i(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_2)\cdot\boldsymbol{r}}+e^{-i\phi}e^{i(R_\phi^*(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_2))\cdot\boldsymbol{r}}+e^{i\phi}e^{i((R_\phi^*)^2(\boldsymbol{q}_1+\boldsymbol{G}+\boldsymbol{b}_2))\cdot\boldsymbol{r}}\right),
\end{aligned}
$$

from which (B.7) follows. □

Proposition B.9. *The operator H^1 maps $L^2_{K,1,-1,A} \to L^2_{K,1,1,B}$, and $L^2_{K,1,-1,B} \to L^2_{K,1,1,A}$.*

The action of H^1 on chiral basis functions is as follows:

$$H^1\chi^{\widetilde{\boldsymbol{q}_1},-1} = \hat{z}_{\boldsymbol{q}_1}\left(\sqrt{3}\chi^{\widetilde{\boldsymbol{0}}} + e^{-i\phi}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{q}_2},1} + e^{i\phi}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{q}_3},1}\right).$$

For all $\boldsymbol{G} \in \Lambda^* \setminus \{\boldsymbol{0}\}$,

$$H^1\chi^{\widetilde{\boldsymbol{G}},-1} = \hat{z}_{\boldsymbol{G}}\left(\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1},1} + e^{-i\phi}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_2},1} + e^{i\phi}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_3},1}\right).$$

For all $\boldsymbol{G} \in \Lambda^*$,

$$H^1\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1},-1} = \hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1}\left(\chi^{\widetilde{\boldsymbol{G}},1} + e^{-i\phi}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_2},1} + e^{i\phi}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_3},1}\right).$$

Proof. The proof is similar to that of Proposition B.8 and is hence omitted. □

Appendix C: Formal expansion of the zero mode

We now bring to bear the developments of the preceding sections on the asymptotic expansion of the zero mode $\psi^\alpha(\boldsymbol{r}) \in L^2_{K,1,1}$ starting from $\Psi^0(\boldsymbol{r}) = e_1(\boldsymbol{r}) = \chi^{\widetilde{\boldsymbol{0}}}(\boldsymbol{r})$. We first give the proof of Proposition IV.1.

Proof of Proposition IV.1. We have seen that $\chi^{\widetilde{\boldsymbol{0}}} \in L^2_{K,1,1}$. By the calculations of the previous section, $H^1\chi^{\widetilde{\boldsymbol{0}}} \in L^2_{K,1,-1}$ which is orthogonal to the null space of H^0. The general solution of $H^0\Psi^1 = -H^1\Psi^0$ is

$$\Psi^1(\boldsymbol{r}) = -P^\perp(H^0)^{-1}P^\perp H^1\Psi^0(\boldsymbol{r}) + C\Psi^0(\boldsymbol{r}),$$

where C is an arbitrary constant, which is in $L^2_{K,1,1}$ by Proposition B.4. To ensure that $\Psi^1(\boldsymbol{r})$ is orthogonal to $\Psi^0(\boldsymbol{r})$ we take $C = 0$. It is clear that this procedure can be repeated to derive an expansion to all orders satisfying the conditions of Proposition IV.1. □

Our goal is to calculate $\Psi^n(\boldsymbol{r}) \in L^2_{K,1,1}$ satisfying the conditions of Proposition B.4 up to $n = 8$. This amounts to calculating, for $n = 1$ to $n = 8$,

$$\Psi^n = -P^\perp(H^0)^{-1}P^\perp H^1\Psi^{n-1}.$$

We do this algorithmically by repeated application of the following proposition, which combines Proposition B.8 and Proposition B.5.

Proposition C.1. *The operator* $-P^{\perp}(H^0)^{-1}P^{\perp}H^1$ *maps* $L^2_{K,1,1,A} \to L^2_{K,1,1,B}$ *and* $L^2_{K,1,1,B} \to L^2_{K,1,1,A}$*. Its action on chiral basis functions is as follows:*

$$-P^{\perp}(H^0)^{-1}P^{\perp}H^1\chi^{\widetilde{\mathbf{0}}} = -\sqrt{3}\overline{\hat{z}_{\boldsymbol{q}_1}}\chi^{\widetilde{\boldsymbol{q}_1},1}, \tag{C.1}$$

and

$$-P^{\perp}(H^0)^{-1}P^{\perp}H^1\chi^{\widetilde{\boldsymbol{q}_1},1} = -\frac{e^{i\phi}\overline{\hat{z}_{\boldsymbol{q}_1-\boldsymbol{q}_2}}}{|\boldsymbol{q}_1-\boldsymbol{q}_2|}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{q}_2},1} - \frac{e^{-i\phi}\overline{\hat{z}_{\boldsymbol{q}_1-\boldsymbol{q}_3}}}{|\boldsymbol{q}_1-\boldsymbol{q}_3|}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{q}_3},1}. \tag{C.2}$$

For all $\boldsymbol{G} \in \Lambda^* \setminus \{\mathbf{0}\}$,

$$\begin{aligned} &-P^{\perp}(H^0)^{-1}P^{\perp}H^1\chi^{\widetilde{\boldsymbol{G}},1} = \\ &-\frac{\overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1}}}{|\boldsymbol{G}+\boldsymbol{q}_1|}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1},1} - \frac{e^{i\phi}\overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_2}}}{|\boldsymbol{G}+\boldsymbol{q}_2|}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_2},1} - \frac{e^{-i\phi}\overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_3}}}{|\boldsymbol{G}+\boldsymbol{q}_3|}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_3},1}. \end{aligned} \tag{C.3}$$

For all $\boldsymbol{G} \in \Lambda^* \setminus \{\mathbf{0}\}$,

$$-P^{\perp}(H^0)^{-1}P^{\perp}H^1\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1},1} = -\frac{\overline{\hat{z}_{\boldsymbol{G}}}}{|\boldsymbol{G}|}\chi^{\widetilde{\boldsymbol{G}},1} - \frac{e^{i\phi}\overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_2}}}{|\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_2|}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_2},1} - \frac{e^{-i\phi}\overline{\hat{z}_{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_3}}}{|\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_3|}\chi^{\widetilde{\boldsymbol{G}+\boldsymbol{q}_1-\boldsymbol{q}_3},1}.$$

We now claim the following.

Proposition C.2. *Let* $\Psi^n(\boldsymbol{r})$ *be the sequence defined by Proposition IV.1. Then*

$$\Psi^1(\boldsymbol{r}) = -\sqrt{3}i\chi^{\widetilde{\boldsymbol{q}_1},1}, \tag{C.4}$$

$$\Psi^2(\boldsymbol{r}) = \left(\frac{\sqrt{3}-i}{2}\right)\chi^{\widetilde{-\boldsymbol{b}_1},1} + \left(\frac{\sqrt{3}+i}{2}\right)\chi^{\widetilde{-\boldsymbol{b}_2},1}, \tag{C.5}$$

$$\Psi^3 = \frac{1}{\sqrt{7}}\left(\frac{\sqrt{7}-3\sqrt{21}i}{14}\right)\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_2},1} + \frac{1}{\sqrt{7}}\left(\frac{-\sqrt{7}-3\sqrt{21}i}{14}\right)\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1},1}, \tag{C.6}$$

$$\begin{aligned} \Psi^4 =& \frac{1}{\sqrt{21}}\left(\frac{-5\sqrt{7}+\sqrt{21}i}{14}\right)\chi^{\widetilde{-\boldsymbol{b}_2},1} + \frac{1}{2\sqrt{21}}\left(\frac{2\sqrt{7}+\sqrt{21}i}{7}\right)\chi^{\widetilde{-2\boldsymbol{b}_2},1} \\ &+ \frac{1}{\sqrt{21}}\left(\frac{-5\sqrt{7}-\sqrt{21}i}{14}\right)\chi^{\widetilde{-\boldsymbol{b}_1},1} + \frac{1}{2\sqrt{21}}\left(\frac{2\sqrt{7}-\sqrt{21}i}{7}\right)\chi^{\widetilde{-2\boldsymbol{b}_1}} \\ &+ \frac{2\sqrt{3}}{21}\chi^{\widetilde{-\boldsymbol{b}_1-\boldsymbol{b}_2},1}, \end{aligned} \tag{C.7}$$

Proof. Equations (C.4) and (C.5) follow immediately from (C.1) and (C.2) and using $\boldsymbol{q}_2 = \boldsymbol{q}_1 + \boldsymbol{b}_1$ and $\boldsymbol{q}_3 = \boldsymbol{q}_1 + \boldsymbol{b}_2$. The derivation of equation (C.6) is more involved, so we give details. Using linearity, and applying (C.3) twice, we find

$$-P^{\perp}(H^0)^{-1}P^{\perp}H^1\Psi^2 =$$
$$\left(\frac{\sqrt{3}-i}{2}\right)\left(\frac{\overline{\hat{z}_{\boldsymbol{q}_1-\boldsymbol{b}_2}}}{|\boldsymbol{q}_1-\boldsymbol{b}_2|}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_2},1}+\frac{e^{i\phi}\overline{\hat{z}_{\boldsymbol{q}_1+\boldsymbol{b}_1-\boldsymbol{b}_2}}}{|\boldsymbol{q}_1+\boldsymbol{b}_1-\boldsymbol{b}_2|}\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-\boldsymbol{b}_2},1}+e^{-i\phi}\overline{\hat{z}_{\boldsymbol{q}_1}}\chi^{\widetilde{\boldsymbol{q}_1},1}\right)$$
$$+\left(\frac{\sqrt{3}+i}{2}\right)\left(\frac{\overline{\hat{z}_{\boldsymbol{q}_1-\boldsymbol{b}_1}}}{|\boldsymbol{q}_1-\boldsymbol{b}_1|}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1},1}+e^{i\phi}\overline{\hat{z}_{\boldsymbol{q}_1}}\chi^{\widetilde{\boldsymbol{q}_1},1}+\frac{e^{-i\phi}\overline{\hat{z}_{\boldsymbol{q}_1+\boldsymbol{b}_2-\boldsymbol{b}_1}}}{|\boldsymbol{q}_1+\boldsymbol{b}_2-\boldsymbol{b}_1|}\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_2-\boldsymbol{b}_1},1}\right).$$

First, the terms proportional to $\chi^{\widetilde{\boldsymbol{q}_1},1}$ cancel. Next, since $R_\phi(\boldsymbol{q}_1+\boldsymbol{b}_1-\boldsymbol{b}_2)=\boldsymbol{q}_1+\boldsymbol{b}_2-\boldsymbol{b}_1$, we have $\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-\boldsymbol{b}_2},1}=\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_2-\boldsymbol{b}_1},1}$. These terms also cancel, leaving (C.6). The derivation of (C.7) (and the higher corrections) is involved but does not depend on any new ideas, and is therefore omitted. □

We give the explicit forms of $\Psi^5(\boldsymbol{r})$-$\Psi^8(\boldsymbol{r})$ in the Supplementary Material.

Remark C.1. *Written out,* (C.4) *and* (C.5) *become*

$$\Psi^1=-\sqrt{3}i\frac{1}{\sqrt{3V}}e_2\left(e^{i\boldsymbol{q}_1\cdot\boldsymbol{r}}+e^{i\boldsymbol{q}_2\cdot\boldsymbol{r}}+e^{i\boldsymbol{q}_3\cdot\boldsymbol{r}}\right),$$

and

$$\Psi^2=-ie^{i\phi}\frac{1}{\sqrt{3V}}e_1\left(e^{i\boldsymbol{b}_1\cdot\boldsymbol{r}}+e^{i(\boldsymbol{b}_2-\boldsymbol{b}_1)\cdot\boldsymbol{r}}+e^{-i\boldsymbol{b}_2\cdot\boldsymbol{r}}\right)+ie^{-i\phi}\frac{1}{\sqrt{3V}}e_1\left(e^{i\boldsymbol{b}_2\cdot\boldsymbol{r}}+e^{-i\boldsymbol{b}_1\cdot\boldsymbol{r}}+e^{i(\boldsymbol{b}_1-\boldsymbol{b}_2)\cdot\boldsymbol{r}}\right),$$

which agree with equation (24) of Tarnopolsky et al.[4] *up to an overall factor of* $\sqrt{V}$ *(this factor cancels in the Fermi velocity so there is no discrepancy).*

Using orthonormality of the chiral basis functions, it is straightforward to calculate the norms of each of the $\Psi^n(\boldsymbol{r})$. We have

Proposition C.3.

$$\|\Psi^0\|=1,\|\Psi^1\|=\sqrt{3},\|\Psi^2\|=\sqrt{2},\|\Psi^3\|=\frac{\sqrt{14}}{7},\|\Psi^4\|=\frac{\sqrt{258}}{42},\|\Psi^5\|=\frac{\sqrt{1968837}}{3458}$$
$$\|\Psi^6\|=\frac{\sqrt{106525799}}{31122},\|\Psi^7\|=\frac{2\sqrt{2129312323981473}}{624696345},\|\Psi^8\|=\frac{\sqrt{183643119755214454}}{4997570760}.$$

Remark C.2. *Note that the sequence of norms of the expansion functions grows much slower than the pessimistic bound* $\|\Psi^{N+1}\|\leq 3\|\Psi^N\|, N=0,1,2,...$ *guaranteed by Proposition IV.2. The reason is that the bounds* (IV.3) *and* (IV.4) *are never attained. As* N *becomes larger,* *the bound* (IV.3) *is very pessimistic because* Ψ^N *is mostly made up of eigenfunctions of* H^0 *with eigenvalues strictly larger than* 1. *The bound* (IV.4) *is also very pessimistic because it is attained only at delta functions, which can only be approximated with a superposition of a large number of eigenfunctions of* H^0. *It seems possible that a sharper bound could be proved starting from these observations, but we do not pursue this in this work.*

We finally give the proof of Proposition IV.4.

Proof of Proposition IV.4. Explicit computation using Proposition B.8 and orthonormality of the chiral basis functions gives

$$\|H^1\Psi^8\| = \frac{\sqrt{4855076200233765642}}{14992712280} \approx 0.147 \leq \frac{3}{20}.$$

□

Appendix D: Proof of Proposition IV.3

We choose Ξ as

$$\Xi := \left\{\begin{matrix} L^2_{K,1}\text{-eigenfunctions of } H^0 \text{ with} \\ \text{eigenvalues with magnitude} \leq 4\sqrt{3} \end{matrix}\right\} \bigcup \left\{ \chi^{\widetilde{\boldsymbol{q}_1 - 4\boldsymbol{b}_1 + \boldsymbol{b}_2}, \pm 1}(\boldsymbol{r}), \chi^{\widetilde{\boldsymbol{q}_1 + \boldsymbol{b}_1 - 4\boldsymbol{b}_2}, \pm 1}(\boldsymbol{r}) \right\}.$$

Part 1. of Proposition IV.3 follows immediately from observing that $\chi^{\widetilde{\boldsymbol{q}_1 - 2\boldsymbol{b}_1 - 2\boldsymbol{b}_2}, \pm 1}$ is not in Ξ but $|\boldsymbol{q}_1 - 2\boldsymbol{b}_1 - 2\boldsymbol{b}_2| = 7$. That $\mu = 7$ is optimal can be seen from Figure D.1.

Part 2. follows from the fact that $\psi^{8,\alpha}(\boldsymbol{r})$ depends only on eigenfunctions of H^0 with eigenvalues with magnitude less than or equal to $4\sqrt{3}$. The largest eigenvalue is $4\sqrt{3}$, coming from dependence of $\Psi^8(\boldsymbol{r})$ on $\chi^{\widetilde{-4\boldsymbol{b}_2}, 1}$, since $|-4\boldsymbol{b}_2| = 4\sqrt{3}$.

Part 3. can be seen from Figure D.1.

Appendix E: Numerical verification of Assumption IV.1

Assumption IV.1 is a lower bound on the smallest magnitude eigenvalues of the 81×81 matrix $Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}$, formed by sandwiching the matrix $P_\Xi H^\alpha P_\Xi$, whose entries are

$$\langle \chi(\boldsymbol{r}) | \, H^\alpha \chi'(\boldsymbol{r}) \rangle \,,$$

where $\langle \cdot | \cdot \rangle$ denotes the L^2_K-inner product, and $\chi(\boldsymbol{r})$ and $\chi'(\boldsymbol{r})$ denote chiral basis functions in Ξ, by the projection $Q^{\alpha,\perp}$. We list the chiral basis functions in Ξ in the supplementary

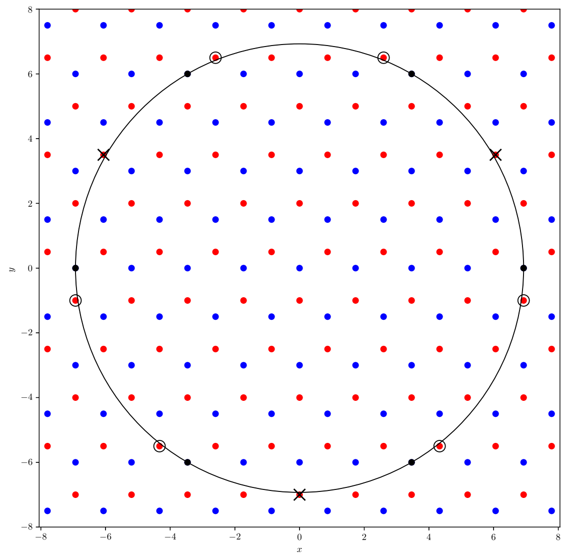

FIG. D.1. Illustration of Ξ in the momentum space lattice. The circle has radius $4\sqrt{3}$, so that every dot within the circle corresponds to two chiral basis vectors included in Ξ. Chiral basis vectors exactly $4\sqrt{3}$ away from the origin, marked with black dots, are also included in Ξ. We also include in Ξ the chiral basis vectors $\left\{\chi^{\widetilde{\boldsymbol{q}_1-4\boldsymbol{b}_1+\boldsymbol{b}_2},\pm1}(\boldsymbol{r}), \chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-4\boldsymbol{b}_2},\pm1}(\boldsymbol{r})\right\}$, which correspond to the dots marked with circles, which are distance 7 (NB. $7 > 4\sqrt{3}$) from the origin. We do not include the chiral basis vectors $\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}$, marked with black crosses, which are also a distance 7 from the origin. The reason for this is so that part 3 of Proposition IV.3 holds. With this choice, every dot in Ξ has *at most one* nearest neighbor lattice point outside of Ξ. It follows immediately from Propositions B.8 and B.9 (H^1 acts by nearest neighbor hopping in the momentum space lattice) that $\|P_\Xi H^1 P_\Xi^\perp\| = 1$. Note that if we chose Ξ to include $\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}$ this would no longer hold because these basis functions would have two nearest neighbors outside Ξ, resulting in the worse bound $\|P_\Xi H^1 P_\Xi^\perp\| \leq \sqrt{2}$.

material. Since $Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}$ anticommutes with $\mathcal{S}$, its spectrum is symmetric about 0. It follows that we can lower bound its smallest magnitude with by directly computing the eigenvalues of the matraix $Q^{\alpha,\perp} P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}$ or by squaring the matrix, finding a lower bound on the eigenvalues of the resulting Hermitian and positive semi-definite matrix, and then taking the square root of that lower bound.

We verify Assumption IV.1 by computing the smallest magnitude eigenvalue by the heevd

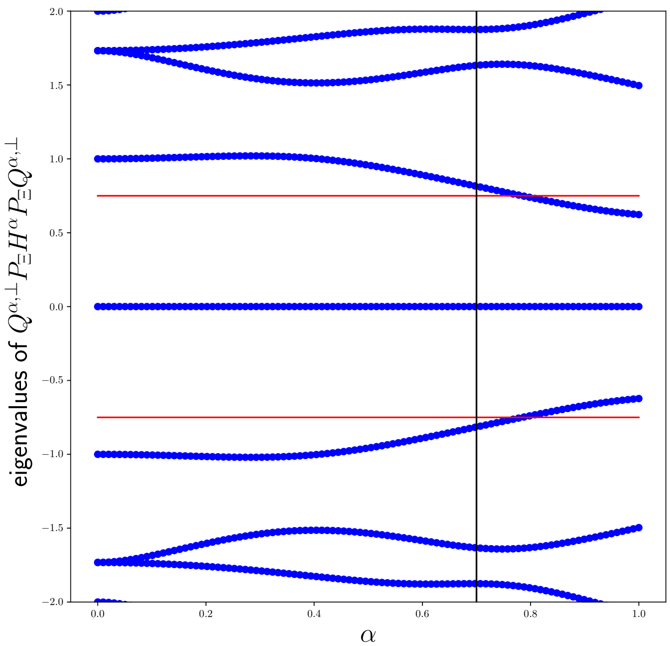

FIG. E.1. Plot of the eigenvalues of $Q^{\alpha,\perp}P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}$ (blue lines), showing the first non-zero eigenvalues are bounded away from 0 by $\frac{3}{4}$ (red lines) when α is less than $\frac{7}{10}$ (black line). The zero eigenvalue corresponds to the subspace spanned by $\psi^{8,\alpha}$ which can be ignored since we are only interested in bounding $Q^{\alpha,\perp}H^\alpha Q^{\alpha,\perp}$ below as a map $Q^{\alpha,\perp}L^2_{K,1} \to Q^{\alpha,\perp}L^2_{K,1}$.

LAPACK routine which uses the divide and conquer algorithm[10], finding that at $\alpha = \frac{7}{10}$, $g^\alpha = 0.81472$ (5sf). The results of a computation of the eigenvalues of $Q^{\alpha,\perp}P_\Xi H^\alpha P_\Xi Q^{\alpha,\perp}$ without squaring are shown in Figure E.1. We obtain the identical result up to 5sf by computing the eigenvalues of the square of the matrix.

Appendix F: Proof of Proposition II.1

We can now prove Proposition II.1. We start by proving (II.12).

1. Proof of (II.12)

We now prove (II.12). It is straightforward to derive

$$\left\langle \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \middle| \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle = \sum_{n=0}^{8}\sum_{j=0}^{n} \left\langle \Psi^j(\boldsymbol{r}) \middle| \Psi^{n-j}(\boldsymbol{r}) \right\rangle \alpha^n + \sum_{n=0}^{7}\sum_{j=0}^{n} \left\langle \Psi^{8-j}(\boldsymbol{r}) \middle| \Psi^{8-(n-j)}(\boldsymbol{r}) \right\rangle \alpha^{16-n}. \tag{F.1}$$

We now make two observations which simplify the computation. First, recall that the operator $-P^\perp (H^0)^{-1} P^\perp H^1$ maps $L^2_{K,1,1,A} \rightarrow L^2_{K,1,1,B}$ and $L^2_{K,1,1,B} \rightarrow L^2_{K,1,1,A}$. It follows that $\Psi^0(\boldsymbol{r}) \in L^2_{K,1,1,A}$, $\Psi^1(\boldsymbol{r}) \in L^2_{K,1,1,B}$, $\Psi^2(\boldsymbol{r}) \in L^2_{K,1,1,A}$, and so on, and hence

$$\left\langle \Psi^{2i}(\boldsymbol{r}) \middle| \Psi^{2j+1}(\boldsymbol{r}) \right\rangle = 0 \quad \forall i, j \in \{0, 1, 2, ...\}.$$

It follows that all terms in (F.1) with odd powers of α vanish. Second, note that since $\Psi^0(\boldsymbol{r}) \in \operatorname{ran} P$ while $\Psi^n(\boldsymbol{r}) \in \operatorname{ran} P^\perp$ for all $n \geq 1$, we have that

$$\left\langle \Psi^n(\boldsymbol{r}) \middle| \Psi^0(\boldsymbol{r}) \right\rangle = \left\langle \Psi^0(\boldsymbol{r}) \middle| \Psi^n(\boldsymbol{r}) \right\rangle = 0 \quad \forall n \in \{1, 2, ...\}.$$

Deriving (II.12) is then just a matter of computation using the properties of the chiral basis. For the leading term, we have

$$\left\langle \Psi^0(\boldsymbol{r}) \middle| \Psi^0(\boldsymbol{r}) \right\rangle = \left\langle \chi^{\widetilde{\boldsymbol{0}}}(\boldsymbol{r}) \middle| \chi^{\widetilde{\boldsymbol{0}}}(\boldsymbol{r}) \right\rangle = 1.$$

For the α^2 term the only non-zero term is

$$\left\langle \Psi^1(\boldsymbol{r}) \middle| \Psi^1(\boldsymbol{r}) \right\rangle = \left\langle -\sqrt{3} i \chi^{\widetilde{\boldsymbol{q}_1,1}}(\boldsymbol{r}) \middle| -\sqrt{3} i \chi^{\widetilde{\boldsymbol{q}_1,1}}(\boldsymbol{r}) \right\rangle = 3,$$

using (C.4). For the α^4 term, the possible non-zero terms are

$$\left\langle \Psi^3(\boldsymbol{r}) \middle| \Psi^1(\boldsymbol{r}) \right\rangle + \left\langle \Psi^2(\boldsymbol{r}) \middle| \Psi^2(\boldsymbol{r}) \right\rangle + \left\langle \Psi^1(\boldsymbol{r}) \middle| \Psi^3(\boldsymbol{r}) \right\rangle,$$

but $\Psi^3(\boldsymbol{r})$ and $\Psi^1(\boldsymbol{r})$ depend on orthogonal chiral basis vectors (see (C.4) and (C.6)) so we are left with

$$\begin{aligned} &\left\langle \Psi^2(\boldsymbol{r}) \middle| \Psi^2(\boldsymbol{r}) \right\rangle \\ &= \left\langle \left(\frac{\sqrt{3} - i}{2} \right) \chi^{\widetilde{-\boldsymbol{b}_1,1}} + \left(\frac{\sqrt{3} + i}{2} \right) \chi^{\widetilde{-\boldsymbol{b}_2,1}} \middle| \left(\frac{\sqrt{3} - i}{2} \right) \chi^{\widetilde{-\boldsymbol{b}_1,1}} + \left(\frac{\sqrt{3} + i}{2} \right) \chi^{\widetilde{-\boldsymbol{b}_2,1}} \right\rangle = 2, \end{aligned}$$

using (C.5) and orthgonality of $\chi^{\widetilde{-\boldsymbol{b}_1,1}}$ and $\chi^{\widetilde{-\boldsymbol{b}_2,1}}$. We omit the derivation of the higher terms since the derivations do not require any new ideas.

2. **Proof of** (II.11)

It is straightforward to derive

$$\left\langle \sum_{n=0}^{8} \alpha^n \Psi^{n*}(-\boldsymbol{r}) \middle| \sum_{n=0}^{8} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle = \sum_{n=0}^{8}\sum_{j=0}^{n} \left\langle \Psi^{j*}(-\boldsymbol{r}) \middle| \Psi^{n-j}(\boldsymbol{r}) \right\rangle \alpha^n + \sum_{n=0}^{7}\sum_{j=0}^{n} \left\langle \Psi^{8-j*}(-\boldsymbol{r}) \middle| \Psi^{8-(n-j)}(\boldsymbol{r}) \right\rangle \alpha^{16-n}. \tag{F.2}$$

We now note the following.

Proposition F.1. *Let $\chi(\boldsymbol{r})$ be a chiral basis function in $L^2_{K,1,1}$. Then $\chi^*(-\boldsymbol{r}) = \chi(\boldsymbol{r})$.*

Proof. The proof follows immediately from the explicit forms of the chiral basis functions in $L^2_{K,1,1}$ given by (B.1)-(B.2)-(B.3) and the observation that for any $\boldsymbol{k} \in \mathbb{R}^2$, $\left(e^{i\boldsymbol{k}\cdot(-\boldsymbol{r})}\right)^* = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$. □

Using Proposition F.1 and the same two observations as in the previous section we have that the only non-zero terms in (F.2) are those with even powers of α, and that other than the leading term, terms involving $\Psi^0(\boldsymbol{r})$ do not contribute. The calculation is then similar to the previous case. For the leading order term we have

$$\left\langle \Psi^{0*}(-\boldsymbol{r}) \middle| \Psi^0(\boldsymbol{r}) \right\rangle = \left\langle \chi^{\widetilde{\boldsymbol{0}}}(\boldsymbol{r}) \middle| \chi^{\widetilde{\boldsymbol{0}}}(\boldsymbol{r}) \right\rangle = 1.$$

The only non-zero α^2 term is

$$\left\langle \Psi^{1*}(-\boldsymbol{r}) \middle| \Psi^1(\boldsymbol{r}) \right\rangle = \left\langle \sqrt{3} i \chi^{\widetilde{\boldsymbol{q}_1},1}(\boldsymbol{r}) \middle| -\sqrt{3} i \chi^{\widetilde{\boldsymbol{q}_1},1}(\boldsymbol{r}) \right\rangle = -3.$$

The only non-zero α^4 term is

$$\begin{aligned}
&\left\langle \Psi^{2*}(-\boldsymbol{r}) \middle| \Psi^2(\boldsymbol{r}) \right\rangle \\
&= \left\langle \left(\frac{\sqrt{3}+i}{2}\right) \chi^{\widetilde{-\boldsymbol{b}_1},1} + \left(\frac{\sqrt{3}-i}{2}\right) \chi^{\widetilde{-\boldsymbol{b}_2},1} \middle| \left(\frac{\sqrt{3}-i}{2}\right) \chi^{\widetilde{-\boldsymbol{b}_1},1} + \left(\frac{\sqrt{3}+i}{2}\right) \chi^{\widetilde{-\boldsymbol{b}_2},1} \right\rangle \\
&= \left(\frac{\sqrt{3}-i}{2}\right)^2 + \left(\frac{\sqrt{3}+i}{2}\right)^2 = 1.
\end{aligned}$$

We omit the derivation of the higher terms since the derivations do not require any new ideas.

Proposition IV.1 implies that the series expansion of $\psi^\alpha(\boldsymbol{r})$ exists up to any order. We can therefore define infinite series by

$$\left\langle \sum_{n=0}^{\infty} \alpha^n \Psi^{n*}(-\boldsymbol{r}) \middle| \sum_{n=0}^{\infty} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle \tag{F.3}$$

$$\left\langle \sum_{n=0}^{\infty} \alpha^n \Psi^{n}(\boldsymbol{r}) \middle| \sum_{n=0}^{\infty} \alpha^n \Psi^n(\boldsymbol{r}) \right\rangle . \tag{F.4}$$

We then have the following.

Proposition F.2. *The expansions* (II.11) *and* (II.12) *approximate the formal series* (F.3) *and* (F.4) *up to terms of order* α^{10}.

Proof. The series agree exactly without any simplifications up to terms of α^9. However, because the even and odd terms in the expansion of $\psi^\alpha(\boldsymbol{r})$ are orthogonal (since they lie in $L^2_{K,1,1,A}$ and $L^2_{K,1,1,B}$ respectively), all terms with odd powers of α vanish in the expansions (F.3)-(F.4). The series may disagree at order α^{10} because the infinite series includes terms arising from inner products of $\Psi^1(\boldsymbol{r})$ and $\Psi^9(\boldsymbol{r})$. □

ACKNOWLEDGMENTS

M.L. and A.W. were supported, in part, by ARO MURI Award No. W911NF-14-0247 and NSF DMREF Award No. 1922165.

REFERENCES

[1] R. Bistritzer and A. H. MacDonald, Proceedings of the National Academy of Sciences of the United States of America **108**, 12233 (2011), arXiv:1009.4203.

[2] P. San-Jose, J. González, and F. Guinea, Physical Review Letters **108**, 1 (2012), arXiv:1110.2883.

[3] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, Nature **556**, 43 (2018).

[4] G. Tarnopolsky, A. J. Kruchkov, and A. Vishwanath, Physical Review Letters **122** (2019), 10.1103/PhysRevLett.122.106405, arXiv:1808.05250.

[5] S. Becker, M. Embree, J. Wittsten, and M. Zworski, "Mathematics of magic angles in a model of twisted bilayer graphene," (2020), arXiv:2008.08489 [math-ph].

[6]G. Catarina, B. Amorim, E. V. Castro, E. V. Castro, E. V. Castro, J. M. V. P. Lopes, J. M. V. P. Lopes, and N. Peres, in *Handbook of Graphene* (Wiley, 2019) pp. 177–231.
[7]A. Meurer, C. P. Smith, M. Paprocki, O. Čertík, S. B. Kirpichev, M. Rocklin, A. Kumar, S. Ivanov, J. K. Moore, S. Singh, T. Rathnayake, S. Vig, B. E. Granger, R. P. Muller, F. Bonazzi, H. Gupta, S. Vats, F. Johansson, F. Pedregosa, M. J. Curry, A. R. Terrel, v. Roučka, A. Saboo, I. Fernando, S. Kulal, R. Cimrman, and A. Scopatz, PeerJ Computer Science **3**, e103 (2017).
[8]T. Kato, *Perturbation theory for linear operators*, Vol. 132 (Springer-Verlag Berlin Heidelberg, 1995).
[9]A. Messiah, *Quantum mechanics: Volume II* (North-Holland Publishing Company Amsterdam, 1962).
[10]E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, *LAPACK Users' Guide*, 3rd ed. (Society for Industrial and Applied Mathematics, Philadelphia, PA, 1999).
[11]S. Carr, S. Fang, Z. Zhu, and E. Kaxiras, Phys. Rev. Research **1**, 13001 (2019).

Appendix G: Supplementary material

We list the chiral basis functions spanning Ξ in Section G 1, list the higher terms in the expansion of the K point wavefunction $\psi^\alpha \in L^2_{K,1,1}$ in Section G 2, and derive the TKV Hamiltonian from the Bistritzer-MacDonald model in Section G 3.

1. Chiral basis functions spanning the subspace Ξ

The chiral basis functions spanning the subspace Ξ are as follows. We note which of the subspaces of H^0 acting on $L^2_{K,1}$ are spanned by the chiral basis vectors at the right.

$\chi^{\widetilde{\mathbf{0}}}$	0 eigenspace
$\chi^{\widetilde{\boldsymbol{q}_1},\pm 1} = \chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1},\pm 1} = \chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_2},\pm 1}$	± 1 eigenspace
$\chi^{\widetilde{-\boldsymbol{b}_1},\pm 1} = \chi^{\widetilde{\boldsymbol{b}_2},\pm 1} = \chi^{\widetilde{\boldsymbol{b}_1-\boldsymbol{b}_2},\pm 1}$	
$\chi^{\widetilde{-\boldsymbol{b}_2},\pm 1} = \chi^{\widetilde{\boldsymbol{b}_1},\pm 1} = \chi^{\widetilde{\boldsymbol{b}_2-\boldsymbol{b}_1},\pm 1}$	$\pm\sqrt{3}$ eigenspace
$\chi^{\boldsymbol{q}_1\widetilde{+\boldsymbol{b}_1+}\boldsymbol{b}_2,\pm 1} = \chi^{\boldsymbol{q}_1\widetilde{+\boldsymbol{b}_1-}\boldsymbol{b}_2,\pm 1} = \chi^{\boldsymbol{q}_1\widetilde{+\boldsymbol{b}_2-}\boldsymbol{b}_1,\pm 1}$	± 2 eigenspace

$$\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_1-\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_2-\boldsymbol{b}_1},\pm1}\qquad \pm\sqrt{7}\ \text{eigenspace}$$

$$\chi^{\widetilde{\boldsymbol{b}_1+\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{b}_2-2\boldsymbol{b}_1},\pm1}$$

$$\chi^{\widetilde{-\boldsymbol{b}_1-\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_2-\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_1-\boldsymbol{b}_2},\pm1}\qquad \pm3\ \text{eigenspace}$$

$$\chi^{\widetilde{-2\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_2-2\boldsymbol{b}_1},\pm1}\qquad \pm2\sqrt{3}\ \text{eigenspace}$$

$$\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1+2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_1+\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_2-2\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_2+2\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_2+\boldsymbol{b}_1},\pm1}\qquad \pm\sqrt{13}\ \text{eigenspace}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1-\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1+3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+3\boldsymbol{b}_1-\boldsymbol{b}_2},\pm1}\qquad \pm4\ \text{eigenspace}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+3\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+3\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+3\boldsymbol{b}_2-2\boldsymbol{b}_1},\pm1}\qquad \pm\sqrt{19}\ \text{eigenspace}$$

$$\chi^{\widetilde{-3\boldsymbol{b}_1+\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_1-3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{b}_1+2\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{-3\boldsymbol{b}_1+2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{b}_1-3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_1+\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{-\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{-2\boldsymbol{b}_1+3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{3\boldsymbol{b}_1-\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{-\boldsymbol{b}_2-2\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{-2\boldsymbol{b}_2+3\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{3\boldsymbol{b}_2-\boldsymbol{b}_1},\pm1}\qquad \pm\sqrt{21}\ \text{eigenspace}$$

$$\chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_1+2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_1-3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_1+2\boldsymbol{b}_2},\pm1}\qquad \pm5\ \text{eigenspace}$$

$$\chi^{\widetilde{-3\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{3\boldsymbol{b}_1-3\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{-3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{3\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{3\boldsymbol{b}_2-3\boldsymbol{b}_1},\pm1}\qquad \pm3\sqrt{3}\ \text{eigenspace}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_1+\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+3\boldsymbol{b}_1-3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1+3\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_1+3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-3\boldsymbol{b}_2},\pm1}\qquad \pm2\sqrt{7}\ \text{eigenspace}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1-\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+4\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1+4\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1+4\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+4\boldsymbol{b}_1-\boldsymbol{b}_2},\pm1}\qquad \pm\sqrt{31}\ \text{eigenspace}$$

$$\chi^{\widetilde{-4\boldsymbol{b}_1+2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_1-4\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{2\boldsymbol{b}_1+2\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{-2\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{4\boldsymbol{b}_1-2\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{-2\boldsymbol{b}_1+4\boldsymbol{b}_2},\pm1}\qquad \pm6\ \text{eigenspace}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_1},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+4\boldsymbol{b}_1-3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+4\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_1+4\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{q}_1+4\boldsymbol{b}_1},\pm1}\qquad \pm\sqrt{37}\ \text{eigenspace}$$

$$\chi^{\widetilde{-4\boldsymbol{b}_1+\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{3\boldsymbol{b}_1-4\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{b}_1+3\boldsymbol{b}_2},\pm1}$$

$$\chi^{\widetilde{-4\boldsymbol{b}_1+3\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{\boldsymbol{b}_1-4\boldsymbol{b}_2},\pm1}=\chi^{\widetilde{3\boldsymbol{b}_1+\boldsymbol{b}_2},\pm1}$$

$$\begin{aligned}
&\chi^{\widetilde{-3\boldsymbol{b}_1-\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{4\boldsymbol{b}_1-3\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{-\boldsymbol{b}_1+4\boldsymbol{b}_2,\pm1}} \\
&\chi^{\widetilde{-3\boldsymbol{b}_1+4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{-\boldsymbol{b}_1-3\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{4\boldsymbol{b}_1-\boldsymbol{b}_2,\pm1}} && \pm\sqrt{39} \text{ eigenspace} \\
&\chi^{\widetilde{\boldsymbol{q}_1-4\boldsymbol{b}_1+2\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{\boldsymbol{q}_1+3\boldsymbol{b}_1-4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_1+3\boldsymbol{b}_2,\pm1}} \\
&\chi^{\widetilde{\boldsymbol{q}_1-4\boldsymbol{b}_1+3\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{\boldsymbol{q}_1+2\boldsymbol{b}_1-4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{\boldsymbol{q}_1+3\boldsymbol{b}_1+2\boldsymbol{b}_2,\pm1}} && \pm\sqrt{43} \text{ eigenspace} \\
&\chi^{\widetilde{-4\boldsymbol{b}_1,\pm1}} = \chi^{\widetilde{4\boldsymbol{b}_1-4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{4\boldsymbol{b}_2,\pm1}} \\
&\chi^{\widetilde{-4\boldsymbol{b}_1+4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{-4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{4\boldsymbol{b}_1,\pm1}} && \pm4\sqrt{3} \text{ eigenspace.}
\end{aligned}$$

We finally add four out of the six modes which span the ±7 eigenspace

$$\begin{aligned}
&\chi^{\widetilde{\boldsymbol{q}_1-4\boldsymbol{b}_1+\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{\boldsymbol{q}_1+4\boldsymbol{b}_1-4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1+4\boldsymbol{b}_2,\pm1}} \\
&\chi^{\widetilde{\boldsymbol{q}_1-4\boldsymbol{b}_1+4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-4\boldsymbol{b}_2,\pm1}} = \chi^{\widetilde{\boldsymbol{q}_1+4\boldsymbol{b}_1+\boldsymbol{b}_2,\pm1}}.
\end{aligned}$$

2. Terms Ψ^5-Ψ^8 in the expansion

Here we list terms Ψ^5-Ψ^8 in the expansion of ψ^α in powers of α. The calculations were assisted by Sympy[7].

$$\begin{aligned}
&\Psi^5 = \\
&\frac{\sqrt{21}}{42}\left(\frac{\sqrt{21}+2\sqrt{7}i}{7}\right)\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_2,1}} + \frac{\sqrt{21}}{42}\left(\frac{-\sqrt{21}+2\sqrt{7}i}{7}\right)\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1,1}} \\
&+ \frac{2\sqrt{3}i}{21}\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-\boldsymbol{b}_2,1}} - \frac{4\sqrt{3}i}{21}\chi^{\widetilde{\boldsymbol{q}_1,1}} - \frac{\sqrt{3}i}{42}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_2-\boldsymbol{b}_1,1}} \\
&+ \frac{\sqrt{273}}{546}\left(\frac{5\sqrt{273}+4\sqrt{91}i}{91}\right)\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-2\boldsymbol{b}_2,1}} + \frac{\sqrt{399}}{798}\left(\frac{2\sqrt{399}-11\sqrt{133}i}{133}\right)\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_2,1}} \\
&+ \frac{\sqrt{273}}{546}\left(\frac{-5\sqrt{273}+4\sqrt{91}i}{91}\right)\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_2-2\boldsymbol{b}_1,1}} + \frac{\sqrt{399}}{798}\left(\frac{-2\sqrt{399}-11\sqrt{133}i}{133}\right)\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1,1}},
\end{aligned}$$

$$\begin{aligned}
&\Psi^6 = \\
&\frac{\sqrt{91}}{42}\left(\frac{9\sqrt{273}-11\sqrt{91}i}{182}\right)\chi^{\widetilde{-\boldsymbol{b}_1,1}} + \frac{4\sqrt{1729}}{5187}\left(\frac{-45\sqrt{5187}-29\sqrt{1729}i}{3458}\right)\chi^{\widetilde{-2\boldsymbol{b}_1,1}} \\
&+\frac{\sqrt{91}}{42}\left(\frac{9\sqrt{273}+11\sqrt{91}i}{182}\right)\chi^{\widetilde{-\boldsymbol{b}_2,1}} - \frac{\sqrt{3}}{26}\chi^{\widetilde{-2\boldsymbol{b}_1+\boldsymbol{b}_2,1}} + \frac{\sqrt{133}}{2394}\left(\frac{9\sqrt{399}-17\sqrt{133}i}{266}\right)\chi^{\widetilde{-3\boldsymbol{b}_1,1}} \\
&+\frac{\sqrt{57}}{798}\left(\frac{59\sqrt{19}-9\sqrt{57}i}{266}\right)\chi^{\widetilde{-2\boldsymbol{b}_1-\boldsymbol{b}_2,1}} + \frac{\sqrt{13}}{546}\left(\frac{-17\sqrt{39}-41\sqrt{13}i}{182}\right)\chi^{\widetilde{-3\boldsymbol{b}_1+\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{57}}{798}\left(\frac{59\sqrt{19}+9\sqrt{57}i}{266}\right)\chi^{\widetilde{-\boldsymbol{b}_1-2\boldsymbol{b}_2,1}} + \frac{4\sqrt{1729}}{5187}\left(\frac{-45\sqrt{5187}+29\sqrt{1729}i}{3458}\right)\chi^{\widetilde{-2\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{133}}{2394}\left(\frac{9\sqrt{399}+17\sqrt{133}i}{266}\right)\chi^{\widetilde{-3\boldsymbol{b}_2,1}} + \frac{\sqrt{13}}{546}\left(\frac{-17\sqrt{39}+41\sqrt{13}i}{182}\right)\chi^{\widetilde{\boldsymbol{b}_1-3\boldsymbol{b}_2,1}},
\end{aligned}$$

$$
\begin{aligned}
&\Psi^7 = \\
&\frac{\sqrt{1032213}}{10374}\left(\frac{-97\sqrt{1032213}-562\sqrt{344071}i}{344071}\right)\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1},1} - \frac{\sqrt{3}i}{42}\chi^{\widetilde{\boldsymbol{q}_1},1} - \frac{2\sqrt{3}i}{273}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1+\boldsymbol{b}_2},1} \\
&+ \frac{\sqrt{3549637}}{217854}\left(\frac{-2621\sqrt{3549637}+1563\sqrt{10648911}i}{7099274}\right)\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1},1} \\
&+ \frac{\sqrt{178087}}{24206}\left(\frac{-241\sqrt{178087}+467\sqrt{534261}i}{356174}\right)\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1+\boldsymbol{b}_2},1} \\
&+ \frac{\sqrt{1032213}}{10374}\left(\frac{97\sqrt{1032213}-562\sqrt{344071}i}{344071}\right)\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_2},1} \\
&+ \frac{\sqrt{178087}}{24206}\left(\frac{241\sqrt{178087}+467\sqrt{534261}i}{356174}\right)\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1+2\boldsymbol{b}_2},1} \\
&+ \frac{\sqrt{4921}}{88578}\left(\frac{-53\sqrt{4921}-75\sqrt{14763}i}{9842}\right)\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_1},1} \\
&+ \frac{2\sqrt{247}}{15561}\left(\frac{-215\sqrt{247}+27\sqrt{741}i}{3458}\right)\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_1+\boldsymbol{b}_2},1} \\
&+ \frac{\sqrt{1767}}{24738}\left(\frac{-10\sqrt{1767}-169\sqrt{589}i}{4123}\right)\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_1-\boldsymbol{b}_2},1} + \frac{2\sqrt{3}i}{2793}\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1-\boldsymbol{b}_2},1} \\
&+ \frac{29\sqrt{3}i}{19110}\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_1+2\boldsymbol{b}_2},1} + \frac{\sqrt{1767}}{24738}\left(\frac{10\sqrt{1767}-169\sqrt{589}i}{4123}\right)\chi^{\widetilde{\boldsymbol{q}_1-\boldsymbol{b}_1-2\boldsymbol{b}_2},1} \\
&+ \frac{\sqrt{3549637}}{217854}\left(\frac{2621\sqrt{3549637}+1563\sqrt{10648911}i}{7099274}\right)\chi^{\widetilde{\boldsymbol{q}_1-2\boldsymbol{b}_2},1} \\
&+ \frac{\sqrt{4921}}{88578}\left(\frac{53\sqrt{4921}-75\sqrt{14763}i}{9842}\right)\chi^{\widetilde{\boldsymbol{q}_1-3\boldsymbol{b}_2},1} \\
&+ \frac{2\sqrt{247}}{15561}\left(\frac{215\sqrt{247}+27\sqrt{741}i}{3458}\right)\chi^{\widetilde{\boldsymbol{q}_1+\boldsymbol{b}_1-3\boldsymbol{b}_2},1},
\end{aligned}
$$

$$
\begin{aligned}
&\Psi^8 = \\
&\frac{\sqrt{160797}}{10374}\left(\frac{-206\sqrt{53599}-61\sqrt{160797}i}{53599}\right)\chi^{\widetilde{-\boldsymbol{b}_1,1}} \\
&+\frac{\sqrt{1694251299}}{1307124}\left(\frac{16249\sqrt{564750433}-10012\sqrt{1694251299}i}{564750433}\right)\chi^{\widetilde{-2\boldsymbol{b}_1,1}} \\
&+\frac{317\sqrt{3}}{11466}\chi^{\widetilde{-\boldsymbol{b}_1-\boldsymbol{b}_2,1}}+\frac{\sqrt{160797}}{10374}\left(\frac{-206\sqrt{53599}+61\sqrt{160797}i}{53599}\right)\chi^{\widetilde{-\boldsymbol{b}_2,1}} \\
&+\frac{67\sqrt{3}}{16758}\chi^{\widetilde{-2\boldsymbol{b}_1+\boldsymbol{b}_2,1}}+\frac{\sqrt{837273}}{620046}\left(\frac{-496\sqrt{279091}-105\sqrt{837273}i}{279091}\right)\chi^{\widetilde{-3\boldsymbol{b}_1,1}} \\
&+\frac{\sqrt{997694607}}{20260422}\left(\frac{5849\sqrt{332564869}-20785\sqrt{997694607}i}{665129738}\right)\chi^{\widetilde{-2\boldsymbol{b}_1-\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{2667}}{13230}\left(\frac{-59\sqrt{889}-5\sqrt{2667}i}{1778}\right)\chi^{\widetilde{-3\boldsymbol{b}_1+\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{1694251299}}{1307124}\left(\frac{16249\sqrt{564750433}+10012\sqrt{1694251299}i}{564750433}\right)\chi^{\widetilde{-2\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{2667}}{13230}\left(\frac{-59\sqrt{889}+5\sqrt{2667}i}{1778}\right)\chi^{\widetilde{-3\boldsymbol{b}_1+2\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{14763}}{1062936}\left(\frac{43\sqrt{4921}-32\sqrt{14763}}{4921}\right)\chi^{\widetilde{-4\boldsymbol{b}_1,1}} \\
&+\frac{\sqrt{114919077}}{39454506}\left(\frac{11413\sqrt{38306359}-2767\sqrt{114919077}i}{76612718}\right)\chi^{\widetilde{-3\boldsymbol{b}_1-\boldsymbol{b}_2,1}} \\
&+\frac{2\sqrt{57}}{46683}\left(\frac{-29\sqrt{19}-31\sqrt{57}i}{266}\right)\chi^{\widetilde{-4\boldsymbol{b}_1+\boldsymbol{b}_2,1}} \\
&+\frac{199\sqrt{3}}{1038996}\chi^{\widetilde{-2\boldsymbol{b}_1-2\boldsymbol{b}_2,1}}-\frac{29\sqrt{3}}{114660}\chi^{\widetilde{-4\boldsymbol{b}_1+2\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{997694607}}{20260422}\left(\frac{5849\sqrt{332564869}+20785\sqrt{997694607}i}{665129738}\right)\chi^{\widetilde{-\boldsymbol{b}_1-2\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{114919077}}{39454506}\left(\frac{11413\sqrt{38306359}+2767\sqrt{114919077}i}{76612718}\right)\chi^{\widetilde{-\boldsymbol{b}_1-3\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{837273}}{620046}\left(\frac{-496\sqrt{279091}+105\sqrt{837273}i}{279091}\right)\chi^{\widetilde{-3\boldsymbol{b}_2,1}} \\
&+\frac{\sqrt{14763}}{1062936}\left(\frac{43\sqrt{4921}+32\sqrt{14763}i}{4921}\right)\chi^{\widetilde{-4\boldsymbol{b}_2,1}}+\frac{2\sqrt{57}}{46683}\left(\frac{-29\sqrt{19}+31\sqrt{57}i}{266}\right)\chi^{\widetilde{\boldsymbol{b}_1-4\boldsymbol{b}_2,1}}
\end{aligned}
$$

3. Derivation of the TKV Hamiltonian from the Bistritzer-MacDonald model

The Bistritzer-MacDonald model of bilayer graphene, with relative twist angle θ, is as follows[1]. Starting from two graphene layers laid exactly on top of each other (i.e., AA stacking configuration), we rotate one layer (call this layer 1) clockwise by $\frac{\theta}{2}$, and the other layer (call this layer 2) counter-clockwise by $\frac{\theta}{2}$. Making the standard Dirac approximation for wavefunctions at the Dirac points, we are lead to the following Hamiltonian describing electrons near to the K-points of the respective layers which are coupled through an "inter-layer coupling potential" $T(\boldsymbol{r})$

$$H = \begin{pmatrix} -iv_0 \boldsymbol{\sigma}_{\theta/2} \cdot \boldsymbol{\nabla} & T(\boldsymbol{r}) \\ T^\dagger(\boldsymbol{r}) & -iv_0 \boldsymbol{\sigma}_{-\theta/2} \cdot \boldsymbol{\nabla} \end{pmatrix}, \tag{G.1}$$

where $\boldsymbol{\sigma}_\theta = e^{-i\frac{\theta}{2}\sigma_3} \boldsymbol{\sigma} e^{i\frac{\theta}{2}\sigma_3}$ and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2)$ is the vector of Pauli matrices, acting on $L^2(\mathbb{R}^2; \mathbb{C}^4)$ with domain $H^1(\mathbb{R}^2; \mathbb{C}^4)$. Note that H ignores possible interactions between electrons with quasi-momentum away from the K-points of each layer, e.g., with the K'-points of each layer. Since the Fermi level occurs at the Dirac energy and interactions between K and K' points are small for small twist angles[6], this is a reasonable simplification. The Hamiltonian (G.1) acts on wavefunctions

$$\psi(\boldsymbol{r}) = \Big(\psi_1^A(\boldsymbol{r}), \psi_1^B(\boldsymbol{r}), \psi_2^A(\boldsymbol{r}), \psi_2^B(\boldsymbol{r})\Big)$$

where $\psi_\tau^\sigma(\boldsymbol{r})$ represents the electron density near to the K point (in momentum space) on sublattice σ and on layer τ.

Under quite general assumptions, the inter-layer coupling has the following form[6]:

$$T(\boldsymbol{r}) = \begin{pmatrix} w_{AA}(e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}) & w_{AB}(e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}}e^{-i\phi} + e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}e^{i\phi}) \\ w_{AB}(e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}}e^{i\phi} + e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}e^{-i\phi}) & w_{AA}(e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}) \end{pmatrix}, \tag{G.2}$$

where

$$\boldsymbol{q}_1 = k_\theta \Big(0, -1\Big), \quad \boldsymbol{q}_{2,3} = \frac{k_\theta}{2}\Big(\pm\sqrt{3}, 1\Big).$$

Here $k_\theta = 2k_D \sin(\theta/2)$ is the distance between the K points of the different layers, and $k_D = |K_1| = |K_2|$ is the distance from the origin to the K point of either layer. Let $\phi := \frac{2\pi}{3}$, then $\boldsymbol{q}_2 = R_\phi \boldsymbol{q}_1$ and $\boldsymbol{q}_3 = R_\phi \boldsymbol{q}_2$ where R_ϕ is the matrix which rotates counterclockwise by ϕ. Note that (G.2) is written in such a way as to show clearly which couplings are between the A lattices of the layers (proportional to w_{AA} and occuring on the diagonal) and between the A and B lattices (proportional to w_{AB} and occuring off the diagonal).

a. Translation and rotation symmetries of the Bistritzer-MacDonald model

The operator H essentially describes coupling on the scale of the bilayer moiré pattern. The moiré lattice vectors are

$$\boldsymbol{a}_1 = \frac{2\pi}{3k_\theta}\left(\sqrt{3}, 1\right), \quad \boldsymbol{a}_2 = \frac{2\pi}{3k_\theta}\left(-\sqrt{3}, 1\right).$$

We denote the moiré lattice generated by these vectors as Λ. It is straightforward to check that H commutes with the "phase-shifted" moiré translation operators

$$\tau_{\boldsymbol{v}} f(\boldsymbol{r}) := \operatorname{diag}(1, 1, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}}, e^{i\boldsymbol{q}_1\cdot\boldsymbol{v}})\tilde{\tau}_{\boldsymbol{v}} f(\boldsymbol{r}), \quad \tilde{\tau}_{\boldsymbol{v}} f(\boldsymbol{r}) = f(\boldsymbol{r}+\boldsymbol{v}),$$

for all $\boldsymbol{v} \in \Lambda$.

The operator also has rotational symmetry. Let R_ϕ be the matrix which rotates vectors by ϕ counter-clockwise

$$R_\phi = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}.$$

Then H commutes with the "phase-shifted" rotation operator

$$\tilde{\mathcal{R}} f(\boldsymbol{r}) := \operatorname{diag}(1, e^{-i\phi}, 1, e^{-i\phi})\mathcal{R} f(\boldsymbol{r}), \quad \mathcal{R} f(\boldsymbol{r}) = f(R_\phi \boldsymbol{r}).$$

b. Deriving TKV from BM

The first step to deriving Tarnopolsky-Kruchkov-Vishwanath's chiral model is to set $w_{AA} = 0$ in the Bistritzer-MacDonald model. Physically, this assumption is motivated by the observation that relaxation effects penalize the AA-stacking configuration, so that one expects[11] $|w_{AA}| \ll |w_{AB}|$.

With this simplification, conjugating $H \to V_\theta H V_\theta^\dagger$ (here † represents the adjoint/Hermitian transpose) by

$$V_\theta := \operatorname{diag}(e^{i\theta/4}, e^{-i\theta/4}, e^{-i\theta/4}, e^{i\theta/4})$$

removes the explicit θ dependence of the Hamiltonian (although H still depends on θ through $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$) so that

$$H = \begin{pmatrix} -iv_0 \boldsymbol{\sigma}_{\theta/2} \cdot \nabla & T_{AB}(\boldsymbol{r}) \\ T_{AB}^\dagger(\boldsymbol{r}) & -iv_0 \boldsymbol{\sigma}_{-\theta/2} \cdot \nabla \end{pmatrix}$$

where

$$T_{AB} = \begin{pmatrix} 0 & w_{AB}(e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}}e^{-i\phi} + e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}e^{i\phi}) \\ w_{AB}(e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}}e^{i\phi} + e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}e^{-i\phi}) & 0 \end{pmatrix}.$$

Conjugating once more $H \to \rho H \rho^\dagger$ by

$$\rho = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

yields

$$H = \begin{pmatrix} 0 & D^\dagger \\ D & 0 \end{pmatrix}, \quad D = \begin{pmatrix} -2iv_0\overline{\partial} & w_{AB}U(\boldsymbol{r}) \\ w_{AB}U(-\boldsymbol{r}) & -2iv_0\overline{\partial} \end{pmatrix},$$

where $\overline{\partial} = \frac{1}{2}(\partial_x + i\partial_y)$ and $U(\boldsymbol{r}) = e^{-i\boldsymbol{q}_1\cdot\boldsymbol{r}} + e^{i\phi}e^{-i\boldsymbol{q}_2\cdot\boldsymbol{r}} + e^{-i\phi}e^{-i\boldsymbol{q}_3\cdot\boldsymbol{r}}$.

After changing variables $\boldsymbol{r} \to k_\theta \boldsymbol{r}$ and re-scaling the $\boldsymbol{q}_i \to \frac{\boldsymbol{q}_i}{k_\theta}, i = 1, 2, 3$, we derive

$$H = \begin{pmatrix} 0 & D^\dagger \\ D & 0 \end{pmatrix}, \quad D = \begin{pmatrix} -2iv_0k_\theta\overline{\partial} & w_{AB}U(\boldsymbol{r}) \\ w_{AB}U(-\boldsymbol{r}) & -2iv_0k_\theta\overline{\partial} \end{pmatrix}.$$

Finally dividing by $v_0 k_\theta$ and defining

$$\alpha := \frac{w_{AB}}{v_0 k_\theta}$$

yields the TKV Hamiltonian stated in the main text.