

DIRAC POINTS FOR TWISTED BILAYER GRAPHENE WITH IN-PLANE MAGNETIC FIELD

SIMON BECKER AND MACIEJ ZWORSKI

ABSTRACT. We study Dirac points of the chiral model of twisted bilayer graphene (TBG) with constant in-plane magnetic field. The striking feature of the chiral model is the presence of perfectly flat bands at *magic angles* of twisting. The Dirac points for zero magnetic field and non magic angles of twisting are fixed at high symmetry points K and K' in the Brillouin zone, with Γ denoting the remaining high symmetry point. For a fixed small constant in-plane magnetic field, we show that as the angle of twisting varies between magic angles, the Dirac points move between K, K' points and the Γ point. In particular, near magic angles, the Dirac points are located near the Γ point. For special directions of the magnetic field, we show that the Dirac points move, as the twisting angle varies, along straight lines and bifurcate orthogonally at distinguished points. At the bifurcation points, the linear dispersion relation of the merging Dirac points disappears and exhibit a quadratic band crossing point (QBCP). The results are illustrated by links to animations suggesting interesting additional structure.

1. INTRODUCTION

Twisted bilayer graphene (TBG) is a material obtained from two sheets of graphene positioned parallel but at a relative twisting angle. It became famous due to an experimentally realized [Ca*18] theoretical prediction [BiMa11] of a *magic* angle of twisting at which TBG acquires special properties. These special properties are due the existence of nearly flat bands of the corresponding periodic spectral problem. Tarnopolsky–Kruchkov–Vishwanath [TKV19] showed that in the chiral model of TBG one obtains exact flat bands with the expectation of a sequence of magic angles converging to 0. That model possesses many attractive mathematical features and was studied by Watson–Luskin [WaLu21] and Becker et al [Be*22, BHZ22a, BHZ22b].

In this paper we consider the effects of a (small) constant magnetic field parallel to TBG, in other words of a constant *in-plane* magnetic field. We follow physics papers Kwan et al [KPS20] and Qin–MacDonald [QiMa21] (see also [RoYa13]) and introduce an additional term $B = B_0 e^{2\pi i \theta}$ to the chiral Hamiltonian. It corresponds to an in-plane magnetic field of strength B_0 and direction $2\pi\theta$ – see (2.1).

The chiral model of TBG is a Hamiltonian which is periodic with respect to the moiré length-scale. Thus, one can study the band structure and finds that the two

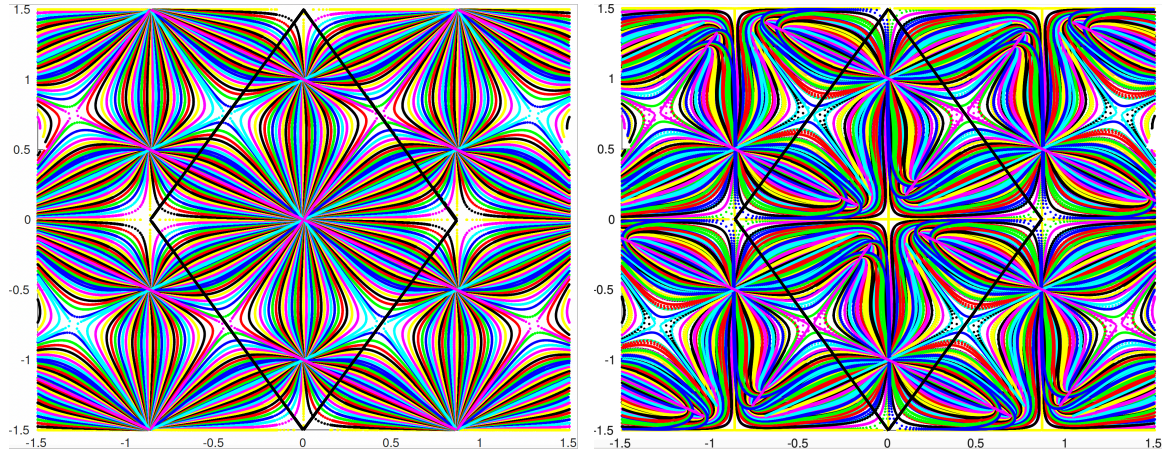


FIGURE 1. We show the movement of Dirac points as α varies in $(0, 2.3)$ for the Bistritzer–MacDonald potential $U(z) = U_{\text{BM}} = \sum_{k=0}^2 \omega^k e^{\frac{1}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}$ (left) and $\alpha \in (0, 2.7)$ and $U(z) = 2^{-\frac{1}{2}}(U_{\text{BM}}(z) - \sum_{k=0}^2 \omega^k e^{-z\bar{\omega}^k - \bar{z}\omega^k})$ (right). (Here we use the convention of [TKV19, Be*22] – see (2.5).) The magnetic field is given by $B = B_0 e^{2\pi i\theta}$ with $B_0 = 0.1$ and curves of different colour correspond to different $\theta \in [0, \frac{1}{2}]$. In the case on the left α passes two simple magic α 's; on the right, it passes two double magic α 's. The Γ point corresponds to 0 and K, K' points to $\pm i$. The boundary of the Brillouin zone, a fundamental domain of Λ^* , is outlined in black. See <https://math.berkeley.edu/~zworski/B01.mp4> and https://math.berkeley.edu/~zworski/B01_double.mp4 for the corresponding animations.

bands closest to zero energy exhibit precisely two Dirac cones at distinguished points in the Brillouin zone, denoted by K and K' . These points, together with another point that we call Γ are distinguished as fixed points under the $2\pi/3$ rotational symmetry of the honeycomb moiré lattice modulo lattice translations. For a discrete set of twisting angles, the so-called magic angles, the bands closest to zero energy become completely flat which we show does no longer happen once an in-plane magnetic field is applied. In this work, we demonstrate that under in-plane magnetic fields the Dirac points are no longer tied to the K and K' points and study their location and structure as the constant magnetic field or the twisting angle are changed. The tunability of the Dirac point locations is particularly rich close to magic angles.

We concentrate on the case of *simple* magic α 's (α is a dimensionless parameter roughly corresponding to the reciprocal of the angle of twisting of the two graphene sheets; see §3.7 for the discussion of simplicity). For the Bistritzer–MacDonald potential $U_{\text{BM}}(z)$ (see the caption to Figure 1) the real magic angles are expected to be simple (see Remark 1 after Theorem 2).

We have the following combination of mathematical and numerical observations:

- We show (Theorem 2) that a small in-plane magnetic field destroys flat bands corresponding to simple magic α 's (under an additional non-degeneracy assumption);
- For small magnetic fields, the motion of Dirac points appears quasi-periodic for $\alpha \in [\alpha_j, \alpha_{j+1}]$ where α_j are the magic angles for the Bistritzer–MacDonald potential [TKV19]. That is most striking for $\theta = 0, \frac{2}{3}$ for which the motion is linear – see Theorem 3 and Figure 6.
- Theorem 1 shows that most of the action takes place near the magic angles: the Dirac points get close to Γ point (Theorem 2; they meet there for $\theta = 0$, Proposition 5.1 and $\theta = \frac{2}{3}$, Proposition 5.3) at simple magic angles – see https://math.berkeley.edu/~zworski/magic_billiard.mp4 for an animation. When the Dirac cones meet, they exhibit a quadratic band crossing point (QBCP), see Figure 3 and Proposition 5.2 (its formulation requires introduction of Bloch–Floquet spectra in §3.1) – for the discussion of such phenomena in the physics literature see [dGGM12, KPS20, MLFP18].
- Figure 2 (right) shows that for fixed α 's and varying directions of the magnetic field, we have “fixed points” at Γ and K, K' with “normal crossings” and the vertices and middle of points of edges of the boundary of the Brillouin zone. These points are precisely the intersection of the rectangles (other than Γ, K, K').
- The situation is more complicated near double (protected) magic angles: see the right panel in Figure 1: at magic α 's, Dirac points are now close to K and K' .

The paper is organized as follows:

- We present the Hamiltonian and the definition of Dirac points in §2. We also establish basic symmetry properties of Dirac points and a perturbation result valid away from magic α 's.
- In §3, we review the theory of magic angles following [Be*22, BHZ22b] but in a more invariant and general way.
- In §4 we set up Grushin problems needed for the understanding the small in-plane magnetic fields as a perturbation.
- We then specialize, in §5, to directions of the magnetic field for which the Dirac points move linearly as α changes. In particular, they meet at special points and we describe the resulting quadratic band crossing.
- We conclude in §6 with the proofs of the main theorems.

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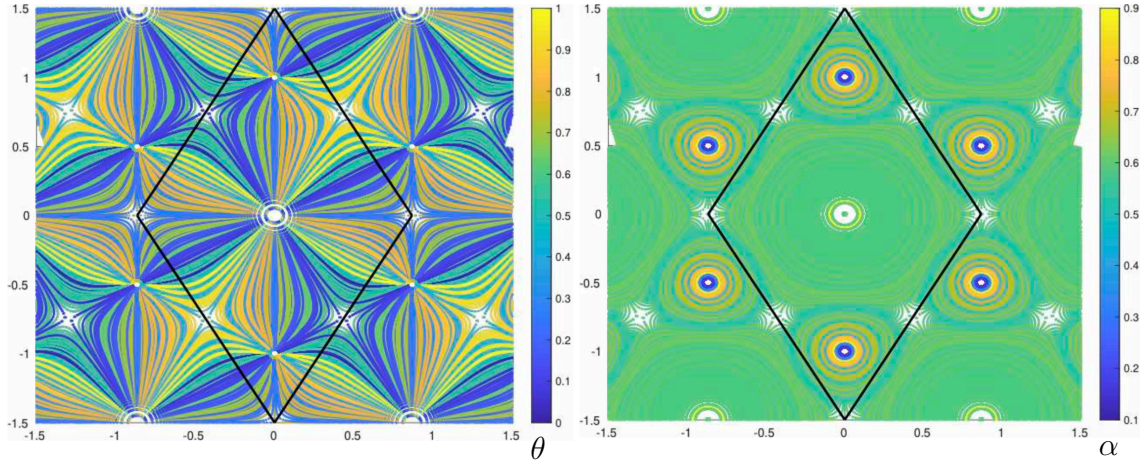


FIGURE 2. The dynamics of Dirac points for the Bistritzer–MacDonald potential $U(z) = U_{\text{BM}} = \sum_{k=0}^2 \omega^k e^{\frac{1}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}$. The magnetic field given by $B = B_0 e^{2\pi i \theta}$ with $B_0 = 0.1$. On the left different colours correspond to different values of θ shown in the colour bar and α varies between 0.1 and 0.9 (this is a colour map version of the left panel of Figure 1). On the right, the colours correspond to different values of α shown in the colour bar and θ varies. The predominance of green (corresponding to the range between 0.5 and 0.6) means that most of the motion happens near the (first) magic alpha – see https://math.berkeley.edu/~zworski/first_band.mp4 for $E_1(\alpha, k) / \max_k E_1(\alpha, k)$ for fixed B as α varies.

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2. IN-PLANE MAGNETIC FIELD

Adding a constant in-plane magnetic field [KPS20, QiMa21] with magnetic vector potential $A = z_{\perp} B \times \hat{e}_{z_{\perp}}$, where z_{\perp} is the coordinate perpendicular to the two-dimensional plane of TBG and $\hat{e}_{z_{\perp}}$ the unit vector pointing in that direction, to the chiral model of TBG [TKV19] results for layers at positions $z_{\perp} = \pm 1$, in the Hamiltonian $H_B(\alpha)$ in (2.7) build from non-normal operators

$$D_B(\alpha) := D(\alpha) + B\sigma_3, \quad D(\alpha) = \begin{pmatrix} 2D_{\bar{z}} & \alpha U(z) \\ \alpha U(-z) & 2D_z \end{pmatrix}, \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (2.1)$$

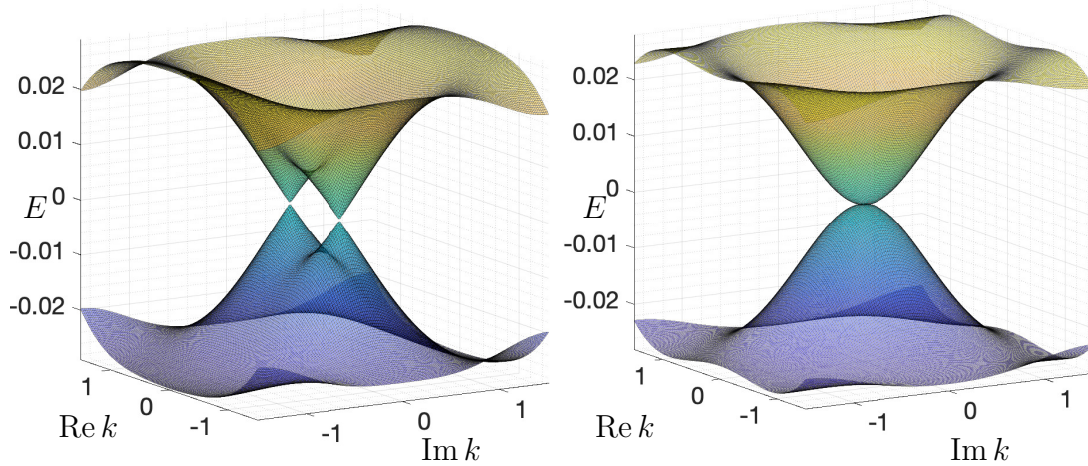


FIGURE 3. When B is real (in the convention of (2.1)), two Dirac cones approach Γ point as $\alpha \rightarrow \alpha^* = \underline{\alpha} + \mathcal{O}(B^3)$ ($\underline{\alpha}$ a simple real magic parameter) on the line $\text{Im } k = 0$ (left). For $\alpha = \alpha^*$, the quasi-momentum k at which the bifurcation happens are the boundary of the Brillouin zone and the Γ -point which is shown in the figure (right). The animation https://math.berkeley.edu/~zworski/Rectangle_1.mp4 shows the motion of Dirac points in this case.

where we make the following assumptions on U :

$$\begin{aligned}
 U(z + \gamma) &= e^{-2i\langle \gamma, K \rangle} U(z), \quad U(\omega z) = \omega U(z), \quad \overline{U(\bar{z})} = -U(-z), \quad \omega = e^{2\pi i/3}, \\
 \gamma \in \Lambda &:= \omega\mathbb{Z} \oplus \mathbb{Z}, \quad \omega K \equiv K \not\equiv 0 \pmod{\Lambda^*}, \quad \Lambda^* := \frac{4\pi i}{\sqrt{3}}\Lambda, \quad \langle z, w \rangle := \text{Re}(z\bar{w}).
 \end{aligned}
 \tag{2.2}$$

In this convention the Bistritzer–MacDonald potential used in [TKV19, Be*22] corresponds to

$$U(z) = -\frac{4}{3}\pi i \sum_{\ell=0}^2 \omega^\ell e^{i\langle z, \omega^\ell K \rangle}, \quad K = \frac{4}{3}\pi.
 \tag{2.3}$$

For a discussion of a perpendicular constant magnetic field in the chiral model of twisted bilayer graphene we refer to [BKZ22].

Remark. We adapt here a more mathematically straightforward convention of coordinates than that of [Be*22, BHZ22a] where we followed [TKV19] (with some, possibly also misguided, small changes; our motivation comes from a cleaner agreement with theta function conventions). The translation between the two conventions is as follows:

the operator considered in [Be*22], and rigorously derived in [CGG22, Wa*22] was

$$\begin{aligned} \tilde{D}(\alpha) &:= \begin{pmatrix} 2D_{\bar{\zeta}} & \alpha U_0(\zeta) \\ \alpha U_0(-\zeta) & 2D_{\bar{\zeta}} \end{pmatrix}, \quad \overline{U_0(\bar{\zeta})} = U_0(\zeta), \\ U_0\left(\zeta + \frac{4\pi i}{3}(a_1\omega + a_2\omega^2)\right) &= \bar{\omega}^{a_1+a_2} U_0(\zeta), \quad U_0(\omega\zeta) = \omega U_0(\zeta). \end{aligned} \quad (2.4)$$

We then have a (twisted) periodicity with respect to $\frac{1}{3}\Gamma$ and periodicity with respect to

$$\Gamma := 4\pi i(\omega\mathbb{Z} + \omega^2\mathbb{Z}) = 4\pi i\Lambda \text{ such that } \Gamma^* := \frac{1}{\sqrt{3}}(\omega\mathbb{Z} \oplus \omega^2\mathbb{Z}) = \frac{\Lambda}{\sqrt{3}}.$$

This means that to switch to (twisted) periodicity with respect to Λ we need a change of variables:

$$\zeta = \frac{4}{3}\pi iz, \quad \frac{1}{3}\Gamma = \frac{4}{3}\pi i\Lambda, \quad 3\Gamma^* = \left(\frac{1}{3}\Gamma\right)^* = \sqrt{3}\Lambda = \frac{3}{4\pi i}\Lambda^*. \quad (2.5)$$

Then

$$\tilde{D}(\alpha) = -\frac{3}{4\pi i} \begin{pmatrix} 2D_{\bar{z}} & \alpha U(z) \\ \alpha U(-z) & 2D_{\bar{z}} \end{pmatrix}, \quad U(z) := -\frac{4}{3}\pi i U_0\left(\frac{4}{3}\pi iz\right). \quad (2.6)$$

The twisted periodicity condition in (2.4) corresponds to the condition in (2.2) since $\bar{\omega}^{a_1+a_2} = e^{i(a_1\omega+a_2\omega^2, K)}$, $K = 4\pi i(-\frac{1}{3} - \frac{2}{3}\omega)/\sqrt{3} = 4\pi/3$. See the caption to Figure 1 for examples of $U_0(z)$ in the coordinates of [TKV19, Be*22].

The self-adjoint Hamiltonian built from (2.1) is given by

$$H_B(\alpha) = \begin{pmatrix} 0 & D_B(\alpha)^* \\ D_B(\alpha) & 0 \end{pmatrix} \quad (2.7)$$

and the Dirac points are given by the spectrum of

$$D_B(\alpha) : H_0^1 \rightarrow L_0^2, \quad L_0^2 := \{u \in L_{\text{loc}}^2(\mathbb{C}; \mathbb{C}) : u(x + \gamma) = \text{diag}(e^{-i\langle \gamma, K \rangle}, e^{i\langle \gamma, K \rangle})u(x)\},$$

with a similar definition of H_0^1 (replace L_{loc}^2 with H_{loc}^1) – see §3.1 for a systematic discussion and explanations.

We recall (see §3.4) that there exists a discrete set $\mathcal{A} \subset \mathbb{C}$ such that

$$\text{Spec}_{L_0^2}(D_0(\alpha)) = \begin{cases} (K + \Lambda^*) \cup (-K + \Lambda^*) & \alpha \notin \mathcal{A} \\ \mathbb{C} & \alpha \in \mathcal{A}. \end{cases} \quad (2.8)$$

The elements of \mathcal{A} are reciprocals of *magic angles* and the real ones are of physical interest. As recalled in Proposition 3.3, elements of \mathcal{A} are characterized by the condition that $\alpha^{-1} \in \text{Spec}_{L_0^2} T_k$, where $\mathbb{C} \setminus \{K, -K\} \mapsto T_k$ is a (holomorphic) family of compact operators given in (3.25) (the spectrum is independent of k and so are its algebraic multiplicities). In this paper we will use the following notion of simplicity (see also §3.7):

$$\alpha \in \mathcal{A} \text{ is said to be simple} \iff 1/\alpha \text{ is a simple eigenvalue of } T_k. \quad (2.9)$$

Here simplicity of an eigenvalue is meant in the algebraic sense.

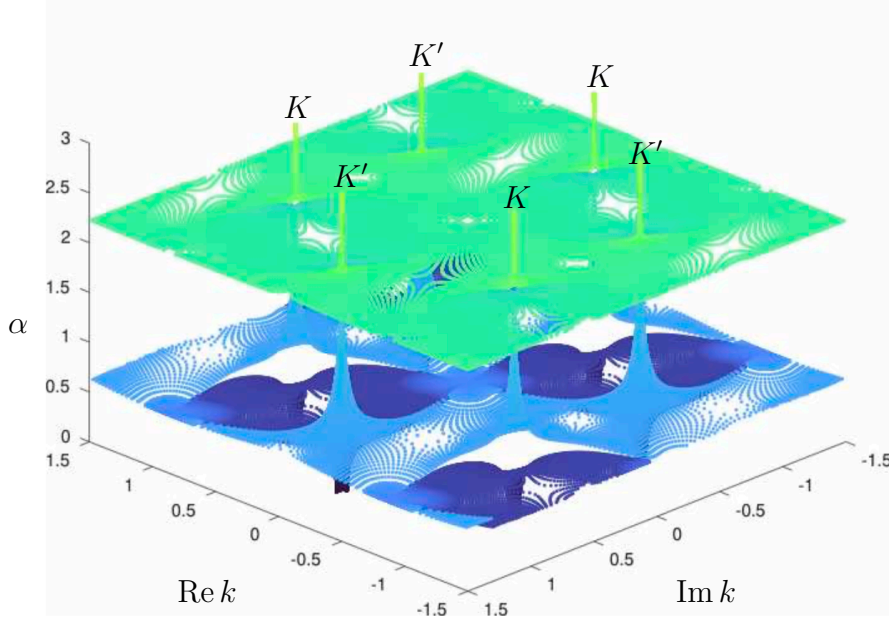


FIGURE 4. Dirac point dynamics for $B = 0.1e^{2\pi i\theta}$ with $\theta \in [0, 1/2]$. Close to the first two magic angles ($\alpha \approx 0.585, 2.221$), the dynamics spreads out in space.

The first result is a consequence of simple perturbation theory and of symmetries of $D_B(\alpha)$:

Theorem 1. *Suppose that $\Omega \Subset \mathbb{C} \setminus \mathcal{A}$ is an open set. Then there exists $\delta = \delta(\Omega)$ such that for $|B| < \delta$ there exists $\alpha \mapsto k_B(\alpha) \in C^\omega(\Omega)$ such that*

$$\text{Spec}_{L_0^2}(D_B(\alpha)) = (k_B(\alpha) + \Lambda^*) \cup (-k_B(\alpha) + \Lambda^*),$$

and $k_B(\alpha) = K + \mathcal{O}(B)$. In addition, for $\alpha, B \in \mathbb{C}$,

$$\begin{aligned} \text{Spec}_{L_0^2} D_{\omega B}(\alpha) &= \omega \text{Spec}_{L_0^2} D_B(\alpha), \\ \text{Spec}_{L_0^2} D_B(-\alpha) &= \text{Spec}_{L_0^2} D_B(\alpha) = -\text{Spec}_{L_0^2} D_B(\alpha), \\ \text{Spec}_{L_0^2} D_{\bar{B}}(\bar{\alpha}) &= \overline{\text{Spec}_{L_0^2} D_B(\alpha)}. \end{aligned} \quad (2.10)$$

Proof of Theorem 1. Proposition 3.3 shows that for $\alpha \in \Omega$ the spectrum of $D(\alpha)$ is given by $\pm K + \Lambda^*$ and for small B we have two eigenvalues for $D_B(\alpha)$. The structure of $D(\alpha)$ implies that

$$\mathcal{E}D(\alpha) = -D(\alpha)\mathcal{E}, \quad \mathcal{E}v(z) := Jv(-z), \quad J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (2.11)$$

and since $J\sigma_3 B = -\sigma_3 B J$ we also have

$$\mathcal{E}(D_B(\alpha) + k)\mathcal{E}^* = -(D_B(\alpha) - k), \quad (2.12)$$

that is the spectrum is invariant under reflection $k \mapsto -k$.

Since $\mathcal{R}D(\alpha)\mathcal{R}^* = \omega D(\alpha)$, $\mathcal{R}u(z) := u(\omega z)$, we have $\mathcal{R}D_B(\alpha)\mathcal{R}^* = \omega D_{\bar{\omega}B}(\alpha)$ which gives the first identity in (2.10). We now recall the following antilinear symmetries:

$$\begin{aligned} FD(\alpha)F &= D(-\bar{\alpha}), \quad Fv(z) := \overline{v(-\bar{z})}, \\ \mathcal{Q}D(\alpha)\mathcal{Q} &= D(-\alpha)^*, \quad Qv(z) := \overline{v(-z)}, \quad \mathcal{Q} := \begin{pmatrix} Q & 0 \\ 0 & -Q \end{pmatrix}. \end{aligned} \quad (2.13)$$

Since $\bullet\sigma_3 B = \sigma_3 B^*\bullet$, $\bullet = F, \mathcal{Q}$, we have

$$F(D_{\bar{B}}(-\bar{\alpha}) - \bar{k})F = (D_B(\alpha) - k) = \mathcal{Q}(D_B(-\alpha)^* - \bar{k})\mathcal{Q}, \quad \mathcal{Q}^2 = F^2 = I,$$

which shows that (since the spectrum is invariant under $k \mapsto -k$),

$$\text{Spec}_{L_0^2}(D_B(\alpha)) = \overline{\text{Spec}_{L_0^2}(D_{\bar{B}}(-\bar{\alpha}))} = \text{Spec}_{L_0^2}(D_B(-\alpha)), \quad (2.14)$$

and that gives the rest of (2.10). \square

We now state a result valid near simple $\underline{\alpha} \in \mathcal{A}$.

Theorem 2. *Suppose $\underline{\alpha} \in \mathcal{A}$ is simple and $g_0(\underline{\alpha}) \neq 0$ where g_0 is defined in (4.5). Then there exists $\delta_0 > 0$ such that for $0 < |B| < \delta_0$ and $|\alpha - \underline{\alpha}| < \delta_0$, the spectrum of $D_B(\alpha)$ on L_0^2 is discrete and*

$$|\text{Spec}_{L_0^2}(D_B(\alpha)) \cap \mathbb{C}/\Lambda^*| = 2, \quad (2.15)$$

where the elements of the spectrum are included according to their (algebraic) multiplicity. In addition, for a fixed constant $a_0 > 0$ and for every ε there exists δ such that for $0 < |B| < \delta$, $|\alpha - \underline{\alpha}| < a_0\delta|B|$,

$$\text{Spec}_{L_0^2}(D_B(\alpha)) \subset \Lambda^* + D(0, \varepsilon), \quad (2.16)$$

where $D(z, \delta) := \{\zeta \in \mathbb{C} : |z - \zeta| < \delta\}$. We also recall that elements of Λ^* , in particular 0, correspond to the Γ point.

Remarks. 1. Existence of the first real magic angle $\underline{\alpha} \simeq 0.585$ was proved by Watson–Luskin [WaLu21] and its simplicity (including the simplicity as an eigenvalue of the operator T_k defined in (3.25)) in [BHZ22a], with computer assistance in both cases. Numerically, the simplicity is valid at the computed real elements of \mathcal{A} for the Bistritzer–MacDonald potential used in [TKV19].

2. The constant $g_0(\alpha)$ can be evaluated numerically (and its non-vanishing for the first magic angles could be established via a computer assisted proof) and here are the results for the (numerically) simple magic angles for the potential U_{BM} in Table 1.

Magic angle $\underline{\alpha}$	0.585	2.221	3.751	5.276	6.794	8.312	9.829
$ g_0(\underline{\alpha}) \simeq$	7e-02	5e-04	7e-04	2e-05	3e-05	9e-07	6e-06
$ g_1(\underline{\alpha}) \simeq$	1.3035	0.2881	0.0880	0.0252	0.0068	0.0017	1.7326e-04

TABLE 1. Values of $g_0(\underline{\alpha})$ defined in (4.5); their non-vanishing is a condition in Theorems 2 and 3. Values $g_1(\underline{\alpha}) = g_1(0, \underline{\alpha})$, defined in (4.7), appear in the perturbation theory in the parameter α . Their non-vanishing is a consequence of the non-vanishing of $g_0(\underline{\alpha})$ as shown in the proof of Proposition 5.1.

3. The combination of Theorems 1 and 2 shows that for any $U \in (\mathbb{C} \setminus \mathcal{A}) \cup \{\alpha\}$ (with $\underline{\alpha}$ satisfying the assumptions of Theorem 2) there exists $\delta = \delta(U)$ such that $0 < |B| < \delta$, the spectrum of $D_B(\alpha)$ is discrete and $|\text{Spec}_{L^2_0}(D_B(\alpha)) \cap \mathbb{C}/\Lambda^*| = 2$.

From the symmetries in (2.10) we conclude that for special values of $\theta = 0, \pm \frac{2}{3}$ the spectrum of $D_B(\alpha)$ has a particularly nice structure as α varies. We state the result for $\theta = 0$, as we can use the first identity in (2.10) to obtain the other two.

Theorem 3. For $0 < B \ll 1$,

$$\text{Spec}_{L^2_0}(D_B(\alpha)) \subset \mathcal{R} := 2\pi(i\mathbb{R} + \mathbb{Z}) \cup \frac{2\pi}{\sqrt{3}}(\mathbb{R} + i\mathbb{Z}), \quad \alpha \in \mathbb{R} \setminus \mathcal{A}. \quad (2.17)$$

Moreover, if the assumptions of Theorem 2 are satisfied at $\underline{\alpha} \in \mathbb{R}$ then for every $\varepsilon > 0$ there are $\delta_0, \delta_1 > 0$ such that

$$\mathcal{R} \setminus \bigcup_{k \in \mathcal{K}_0} D(k, \varepsilon) \subset \bigcup_{\underline{\alpha} - \delta_1 < \alpha < \underline{\alpha} + \delta_1} \text{Spec}_{L^2_0}(D_B(\alpha)) \subset \mathcal{R}, \quad 0 < B < \delta_0. \quad (2.18)$$

Here, $D(z, \delta) := \{\zeta \in \mathbb{C} : |z - \zeta| < \delta\}$ and $\mathcal{K}_0 = \{K, -K\} + \Lambda^*$, $K = \frac{4}{3}\pi$, the set of protected states in the Brillouin zone for the non-magnetic model, defined in Proposition 3.2. In addition, for every $k \in \mathcal{R} \setminus \bigcup_{k \in \mathcal{K}_0} D(k, \varepsilon)$ there is a unique $\alpha \in (\underline{\alpha} - \delta_1 < \alpha < \underline{\alpha} + \delta_1)$ such that $k \in \text{Spec}_{L^2_0}(D_B(\alpha))$.

Remarks. 1. A more precise statement about the behaviour at \mathcal{R} is given in Propositions 5.1 and 5.3 – the implicit formulas for $\lambda = 1/\alpha$ in terms of k and B describe a bifurcation phenomenon. In particular, when B is real, the bifurcation of the eigenvalues of $D_B(\alpha)$ at 0 (at the specific value of α) is given by (5.5). For the bifurcation at the vertices of the boundary of the Brillouin zone, see (5.18).

2. The inclusion (2.17) means that the spectrum lies on a grid of straight lines parallel to the x and y axes – see https://math.berkeley.edu/~zworski/Rectangle_1.mp4. To obtain the sets of other rectangles we use the the first identity in (2.10), that is take $B = \omega B_0$, $B_0 > 0$.

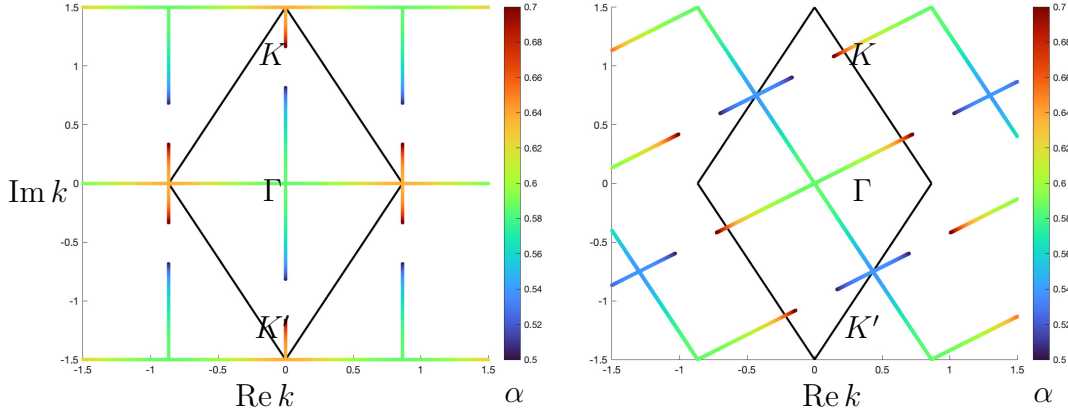


FIGURE 5. Dirac point trajectory for $B = 0.1$ (left) and $B = 0.1\omega$ (right). The bifurcation happens at Γ and one additional point (modulo Λ^*) in each figure, respectively. The colors indicate the position of the Dirac cones for given values of α . The exclusion of K and K' points in the statement of Theorem 3 seems to be a technical issue, as shown in https://math.berkeley.edu/~zworski/Rectangle_2.mp4 (for the case of the figure on the right).

3. REVIEW OF MAGIC ANGLE THEORY

We start with a general discussion of operators arising in chiral TBG models.

3.1. Bloch–Floquet theory. We recall that

$$\Lambda := \mathbb{Z} \oplus \omega\mathbb{Z}, \quad \omega := e^{2\pi i/3}, \quad \omega\Lambda = \Lambda, \quad \Lambda^* = \frac{4\pi i}{\sqrt{3}}\Lambda.$$

(The dual basis of $\{1, \omega\}$ is given by $\{-4\pi i\omega/\sqrt{3}, 4\pi i/\sqrt{3}\}$.)

We then consider a generalization of (2.1):

$$D(\alpha) := 2D_z + \alpha V(z) : H_{\text{loc}}^1(\mathbb{C}; \mathbb{C}^n) \rightarrow L_{\text{loc}}^2(\mathbb{C}; \mathbb{C}^n), \quad H(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* \\ D(\alpha) & 0 \end{pmatrix},$$

where $V(z) := C^\infty(\mathbb{C}; \mathbb{C}^n \otimes \mathbb{C}^n)$. Let $\rho : \Lambda \rightarrow U(n)$ be a unitary representation and assume that

$$V(z + \gamma) = \rho(\gamma)^{-1}V(z)\rho(\gamma). \quad (3.1)$$

We note that without loss of generality (amounting to a basis change on \mathbb{C}^n) we can assume that

$$\rho(\gamma) = \text{diag} [(\chi_{k_j}(\gamma))_{j=1}^n], \quad k_j \in \mathbb{C}/\Lambda^*, \quad \chi_k(\gamma) := \exp(i\langle \gamma, k \rangle). \quad (3.2)$$

If in the corresponding basis, $V(z) = (V_{ij}(z))_{0 \leq i, j \leq k}$, then (3.1) means that

$$V_{ij}(z + \gamma) = \exp(i\langle \gamma, k_j - k_i \rangle) V_{ij}(z). \quad (3.3)$$

If we define

$$\rho(z) := \text{diag} \left[(e^{i\langle z, k_j \rangle})_{j=1}^n \right],$$

then

$$V_\rho(z + \gamma) = V_\rho(z), \quad V_\rho(z) := \rho(z)V(z)\rho(z)^{-1},$$

and

$$\rho(z)D(\alpha)\rho(z)^{-1} = D_\rho(\alpha), \quad D_\rho(\alpha) := \text{diag} \left[(2D_{\bar{z}} - k_j)_{j=1}^n \right] + V_\rho(z), \quad (3.4)$$

which is a periodic operator. In view of this standard Bloch-Floquet theory applies, which can be presented using modified translations:

$$\mathcal{L}_\gamma u(z) := \rho(\gamma)u(z + \gamma), \quad \mathcal{L}_\gamma : \mathcal{S}'(\mathbb{C}, \mathbb{C}^n) \rightarrow \mathcal{S}'(\mathbb{C}, \mathbb{C}^n).$$

We have

$$\mathcal{L}_\gamma D(\alpha) = D(\alpha)\mathcal{L}_\gamma.$$

Thus, we can define a generalized Bloch transform

$$\begin{aligned} \mathcal{B}u(z, k) &:= \sum_{\gamma \in \Lambda} e^{i\langle z + \gamma, k \rangle} \mathcal{L}_\gamma u(z), \quad \sigma_3 \mathcal{B}u(z, k + p) = e^{i\langle z, p \rangle} \sigma_3 \mathcal{B}u(z, k), \quad p \in \Lambda^*, \quad u \in \mathcal{S}(\mathbb{C}), \\ \mathcal{L}_\alpha \mathcal{B}u(\bullet, k) &= \sum_{\gamma} e^{i\langle z + \alpha + \gamma, k \rangle} \mathcal{L}_{\alpha + \gamma} u(z) = \sigma_3 \mathcal{B}u(\bullet, k), \quad \alpha \in \Lambda \end{aligned}$$

such that (extending the actions of \mathcal{L}_γ and $\sigma_3 B$ to $\mathbb{C}^n \times \mathbb{C}^n$ -valued functions diagonally)

$$\begin{aligned} \sigma_3 B D(\alpha) &= (D(\alpha) - k) \sigma_3 B, \quad D(\alpha) - k = e^{i\langle z, k \rangle} D(\alpha) e^{-i\langle z, k \rangle}, \\ \sigma_3 B H(\alpha) &= H_k(\alpha) \sigma_3 B, \quad H_k(\alpha) := e^{i\langle z, k \rangle} H(\alpha) e^{-i\langle z, k \rangle} = \begin{pmatrix} 0 & D(\alpha)^* - \bar{k} \\ D(\alpha) - k & 0 \end{pmatrix}. \end{aligned} \quad (3.5)$$

We check that

$$\int_{\mathbb{C}/\Lambda} \int_{\mathbb{C}/\Lambda^*} |\sigma_3 \mathcal{B}u(z, k)|^2 dm(z) dm(k) = |\mathbb{C}/\Lambda^*| \int_{\mathbb{C}} |u(z)|^2 dm(z),$$

and that

$$\mathcal{C}v(z) := |\mathbb{C}/\Lambda^*|^{-1} \int_{\mathbb{C}/\Lambda^*} v(z, k) e^{-i\langle z, k \rangle} dm(k)$$

is the inverse of $\sigma_3 B$. We now define

$$H_0^s = H_0^s(\mathbb{C}; \mathbb{C}^k) := \{u \in H_{\text{loc}}^s(\mathbb{C}; \mathbb{C}^k) : \mathcal{L}_\gamma u = u, \gamma \in \Lambda\}, \quad L_0^2 := H_0^0, \quad k = n, 2n,$$

We have a unitary operator identifying L_0^2 with $L^2(\mathbb{C}/\Lambda)$

$$\mathcal{U}_0 u(z) := \rho(z)u(z), \quad \mathcal{U}_0 : L_0^2 \rightarrow L^2(\mathbb{C}/\Lambda; \mathbb{C}^n), \quad \mathcal{U}_0 D(\alpha) \mathcal{U}_0^* = D_\rho(\alpha), \quad (3.6)$$

where we used the notation of (3.4).

In view of this, $\text{Spec}_{L_0^2}(H_k(\alpha))$ (with the domain given by H_0^1) is discrete and

$$\text{Spec}_{L^2(\mathbb{C}; \mathbb{C}^{2n})}(H(\alpha)) = \bigcup_{k \in \mathbb{C}/\Lambda^*} \text{Spec}_{L_0^2} H_k(\alpha).$$

Since for $p \in \Lambda^*$,

$$\tau(p) : L_0^2 \rightarrow L_0^2, \quad [\tau(p)u](z) := e^{i\langle z, p \rangle} u(z), \quad \tau(p)^{-1} = \tau(p)^*, \quad (3.7)$$

and

$$\tau(p)^* D(\alpha) \tau(p) = D(\alpha) + p,$$

we have

$$\text{Spec}_{L_0^2} D(\alpha) = \text{Spec}_{L_0^2} D(\alpha) + \Lambda^*. \quad (3.8)$$

Finally, we use (3.4) and $\text{Spec}_{L^2(\mathbb{C}/\Lambda; \mathbb{C})}(2D_{\bar{z}}) = \Lambda^*$ (with simple eigenvalues) to see that (for ρ given by (3.2)) we have the disjoint union

$$\text{Spec}_{L_0^2}(2D_{\bar{z}}) = \bigsqcup_{j=1}^n (\Lambda^* - k_j), \quad \text{Domain of } 2D_{\bar{z}} = H_0^1. \quad (3.9)$$

3.2. Rotational symmetries. We now introduce

$$\Omega u(z) := u(\omega z), \quad u \in \mathcal{S}'(\mathbb{C}; \mathbb{C}^n),$$

and in addition to (3.1) assume that

$$V(\omega z) = \omega V(z). \quad (3.10)$$

(We do not have many options here as $\Omega D_{\bar{z}} = \omega D_{\bar{z}} \Omega$). Then

$$\Omega D(\alpha) = \omega D(\alpha) \Omega,$$

and

$$\mathcal{C} H(\alpha) = H(\alpha) \mathcal{C}, \quad \mathcal{C} := \begin{pmatrix} \Omega & 0 \\ 0 & \bar{\omega} \Omega \end{pmatrix} : \mathcal{S}'(\mathbb{C}; \mathbb{C}^n \times \mathbb{C}^n) \rightarrow \mathcal{S}'(\mathbb{C}; \mathbb{C}^n \times \mathbb{C}^n).$$

We have the following commutation relation

$$\begin{aligned} \mathcal{L}_\gamma \Omega u(z) &= \rho(\gamma) u(\omega(z + \gamma)) = \rho(\gamma - \omega\gamma) \rho(\omega\gamma) u(\omega z + \omega\gamma) \\ &= \rho(\gamma - \omega\gamma) \Omega \mathcal{L}_{\omega\gamma} u(z). \end{aligned}$$

A natural case to consider is given by

$$\rho(\gamma) = \rho(\omega\gamma), \quad \forall \gamma \in \Lambda, \quad (3.11)$$

which implies that

$$\rho(\gamma)^3 = \rho(\gamma + \omega\gamma + \omega^2\gamma) = \rho(0) = I_{\mathbb{C}^n}. \quad (3.12)$$

In the notation of (3.2), condition (3.11) means that

$$\bar{\omega} k_j \equiv k_j \pmod{\Lambda^*} \iff k_j \in \mathcal{K} := \frac{4\pi i}{\sqrt{3}} (\{0, \pm(\frac{1}{3} + \frac{2}{3}\omega)\} + \Lambda). \quad (3.13)$$

We see that \mathcal{K}/Λ^* is the subgroup of fixed points of multiplication $\omega : \mathbb{C}/\Lambda^* \rightarrow \mathbb{C}/\Lambda^*$ and it is isomorphic to \mathbb{Z}_3 .

Since (3.11) implies that

$$\mathcal{L}_\gamma \Omega = \Omega \mathcal{L}_{\omega\gamma}, \quad \mathcal{L}_\gamma \mathcal{C} = \mathcal{C} \mathcal{L}_{\omega\gamma}, \quad \mathcal{C} \mathcal{L}_\gamma = \mathcal{L}_{\bar{\omega}\gamma} \mathcal{C},$$

we follow [Be*22, §2.1] and combine the two actions into a group of unitary action which commute with $H(\alpha)$:

$$\begin{aligned} G := \Lambda \rtimes \mathbb{Z}_3, \quad \mathbb{Z}_3 \ni \ell : \gamma \rightarrow \bar{\omega}^\ell \gamma, \quad (\gamma, \ell) \cdot (\gamma', \ell') &= (\gamma + \bar{\omega}^\ell \gamma', \ell + \ell'), \\ (\gamma, \ell) \cdot u &= \mathcal{L}_\gamma \mathcal{C}^\ell u, \quad u \in L^2_{\text{loc}}(\mathbb{C}; \mathbb{C}^n \times \mathbb{C}^n). \end{aligned} \quad (3.14)$$

By taking a quotient by 3Λ we obtain a finite group which acts unitarily on $L^2(\mathbb{C}/3\Lambda)$, and that action commutes with $H(\alpha)$:

$$G_3 := G/3\Lambda = \Lambda/3\Lambda \rtimes \mathbb{Z}_3 \simeq \mathbb{Z}_3^2 \rtimes \mathbb{Z}_3. \quad (3.15)$$

By restriction to the first two components, G and G_3 act on \mathbb{C}^n -valued function and use the same notation for those actions.

The key fact (hence the name *chiral model*) is that

$$\begin{aligned} H(\alpha) &= -\mathcal{W} H(\alpha) \mathcal{W}, \quad \mathcal{W} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} : \mathbb{C}^n \times \mathbb{C}^n \rightarrow \mathbb{C}^n \times \mathbb{C}^n, \\ \mathcal{W} \mathcal{C} &= \mathcal{C} \mathcal{W}, \quad \mathcal{L}_\gamma \mathcal{W} = \mathcal{W} \mathcal{L}_\gamma. \end{aligned} \quad (3.16)$$

3.3. Protected states. We now make the assumption (3.11) and consider the question of protected states. We are looking for the set $\mathcal{K}_0 \subset \mathbb{C}$ such that

$$\forall \alpha \in \mathbb{C}, k \in \mathcal{K}_0, \quad 0 \in \text{Spec}_{L^2_0} H_k(\alpha). \quad (3.17)$$

This condition is equivalent to

$$k \in \text{Spec}_{L^2_0} D(\alpha) \iff k \in \text{Spec}_{L^2(\mathbb{C}/\Lambda; \mathbb{C}^n)} D_\rho(\alpha),$$

where we used the notation of (3.4). Putting $\alpha = 0$ we see that $\mathcal{K}_0 \subset \mathcal{K}$.

The following simple lemma is used a lot. To formulate it we introduce the following spaces:

$$H_k^s := \{u \in H^s(\mathbb{C}/3\Lambda; \mathbb{C}^2 \times \mathbb{C}^2) : \mathcal{L}_\gamma u = e^{i\langle k, \gamma \rangle} u\}, \quad k \in \mathcal{K}/\Lambda^* \simeq \mathbb{Z}^3, \quad p \in \mathbb{Z}^3, \quad (3.18)$$

(with the corresponding definition of L_k^2).

Lemma 3.1. *Suppose that $k, k' \in \mathcal{K}$ and $\tau(k)$ is defined as in (3.7). Then in the notation of (3.18), $\tau(k) : H_{k'}^s \rightarrow H_{k'+k}^s$ and*

$$\begin{aligned} \tau(k) : \ker_{H_0^1}(D(\alpha) + k) &\rightarrow \ker_{H_k^1} D(\alpha), \\ \tau(k) : \ker_{H_0^1} H_{-k}(\alpha) &\rightarrow \ker_{H_k^1} H(\alpha). \end{aligned} \quad (3.19)$$

Proof. We have $\tau(k) = e^{i\langle k, z \rangle}$ (as a multiplication operator) and for $u \in H_{k'}^s$,

$$\mathcal{L}_\gamma(\tau(k)u)(z) = e^{i\langle k, z + \gamma \rangle} \mathcal{L}_\gamma u(z) = e^{i\langle k+k', \gamma \rangle} \tau(k)u(z),$$

which proves the mapping property of $\tau(k)$. Also, $D(\alpha)w = e^{i\langle z, k \rangle} (D(\alpha) + k)(e^{-i\langle z, k \rangle} w)$. Hence if $(D(\alpha) + k)u = 0$ and $\mathcal{L}_\gamma u = u$ then $w := e^{i\langle z, k \rangle} u \in H^1(\mathbb{C}/3\Lambda; \mathbb{C}^{2n})$, $D(\alpha)w = 0$, and $\mathcal{L}_\gamma w = \mathcal{L}_\gamma(e^{i\langle z, k \rangle} u) = e^{i\langle z + \gamma, k \rangle} \mathcal{L}_\gamma u = e^{i\langle \gamma, k \rangle} w$, that is $w \in H_k^1$. \square

We are interested in the case of $n = 2$ and obtain the following reinterpretation of earlier protected states statements – see [TKV19].

Proposition 3.2. *If $n = 2$ (in the notation of (3.2) and (3.17)) and $k_1 \not\equiv k_2 \pmod{\Lambda^*}$, $k_j \in \mathcal{K}$, then $\mathcal{K}_0 = \{-k_1, -k_2\} + \Lambda^*$.*

Proof. We use (3.19) and decompose $\ker_{H^1(\mathbb{C}/3\Lambda; \mathbb{C}^4)} H(\alpha)$ into representations of G_3 given by (3.14). From (3.16) we see that the spectrum of $H(\alpha)$ restricted to a representation of G_3 is symmetric with respect to the origin. If (see [Be*22, §2.2] for a review of representations of G_3)

$$H_{k,p}^s := \{u \in H^s(\mathbb{C}/3\Lambda; \mathbb{C}^2 \times \mathbb{C}^2) : \mathcal{L}_\gamma \mathcal{C}^\ell u = e^{i\langle k, \gamma \rangle} \bar{\omega}^{\ell p} u\}, \quad (3.20)$$

$k \in \mathcal{K}/\Lambda^* \simeq \mathbb{Z}_3$, $p \in \mathbb{Z}_3$, (with the corresponding definition of $L_{k,p}^2$) then the constant functions (given by the standard basis vectors in \mathbb{C}^4) satisfy

$$\mathbf{e}_1 \in H_{k_1,0}^1, \quad \mathbf{e}_2 \in H_{k_2,0}^1, \quad \mathbf{e}_3 \in H_{k_1,1}^1, \quad \mathbf{e}_4 \in H_{k_2,1}^1,$$

and since $k_1 \not\equiv k_2 \pmod{\Lambda^*}$, all these spaces are different. The spectrum of $H(\alpha)|_{L_{k,p}^2}$ is even (see (3.16)) and $\ker_{H_{k_j,p}^1} H(0) = \mathbb{C} \mathbf{e}_{j+2p}$, $j = 1, 2$, $p = 0, 1$. Continuity of eigenvalues shows that

$$\dim \ker_{L_{k_j,p}^2} H(\alpha) \geq 1, \quad \alpha \in \mathbb{C}, \quad j = 1, 2, \quad p = 0, 1. \quad (3.21)$$

which in view of Lemma 3.1 concludes the proof. \square

Remark. Under the assumptions of Proposition 3.2 the corresponding $-k_1, -k_2 \in \mathbb{C}/\Lambda^*$ are called the K and K' points in the physics literature. The remaining element of \mathcal{K}/Λ^* is called the Γ point.

Existence of protected states shows that we have a natural labelling for the eigenvalues of $H(k)$ on L_0^2 :

$$\begin{aligned} \text{Spec}_{L_0^2}(H(k)) &= \{E_j(\alpha, k)\}_{j \in \mathbb{Z}^*}, \quad E_j(\alpha, k) = -E_{-j}(\alpha, k), \\ 0 \leq E_1(\alpha, k) &\leq E_2(\alpha, k) \leq \dots, \quad E_{\pm 1}(\alpha, -k_1) = E_{\pm 1}(\alpha, -k_2) = 0. \end{aligned} \quad (3.22)$$

where the eigenvalues are included according to their multiplicities (and $\mathbb{Z}^* := \mathbb{Z} \setminus \{0\}$).

3.4. Magic angles. We recall the main result of [Be*22], the spectral characterization of *magic angles*. See also proof of [BHZ22b, Proposition 2.2].

Proposition 3.3. *Suppose that $n = 2$ and that the condition (3.11) holds. Then, in the notation of Proposition 3.2 there exists a discrete set \mathcal{A} such that*

$$\text{Spec}_{L_0^2} D(\alpha) = \begin{cases} \mathcal{K}_0 & \alpha \notin \mathcal{A}, \\ \mathbb{C} & \alpha \in \mathcal{A}. \end{cases} \quad (3.23)$$

Moreover,

$$\alpha \in \mathcal{A} \iff \exists k \notin \mathcal{K}_0, \alpha^{-1} \in \text{Spec}_{L_0^2} T_k \iff \forall k \notin \mathcal{K}_0, \alpha^{-1} \in \text{Spec}_{L_0^2} T_k, \quad (3.24)$$

where T_k is a compact operator given by

$$T_k := R(k)V(z) : L_0^2 \rightarrow L_0^2, \quad R(k) := (2D_{\bar{z}} - k)^{-1} \quad (3.25)$$

3.5. Antilinear symmetry. We will make the following assumption:

$$\mathcal{A}D(\alpha) = -D(\alpha)^*\mathcal{A}, \quad \mathcal{A} := \begin{pmatrix} 0 & \Gamma \\ -\Gamma & 0 \end{pmatrix}, \quad \Gamma v(z) = \overline{v(z)}. \quad (3.26)$$

A calculation based on the definition of \mathcal{L}_γ gives

$$\mathcal{A} : L_{k,p}^2 \rightarrow L_{-k+k_1+k_2,-p}^2, \quad k \in \mathcal{K}, \quad p \in \mathbb{Z}_3. \quad (3.27)$$

In particular if (as we assume) $k_1 \not\equiv k_2 \pmod{\Lambda^*}$ and $k_0 \notin \{k_1, k_2\} + \Lambda^*$, then $-k_0 + k_1 + k_2 \equiv k_0 \pmod{\Lambda^*}$, and consequently

$$\mathcal{A} : L_{k_0,p}^2 \rightarrow L_{k_0,-p}^2, \quad p \in \mathbb{Z}_3. \quad (3.28)$$

Since (we put $\alpha = 1$ to streamline notation; that amounts to absorbing α into V)

$$\mathcal{A} \begin{pmatrix} V_{11} & 0 \\ 0 & V_{22} \end{pmatrix} = - \begin{pmatrix} -\bar{V}_{22} & 0 \\ 0 & -\bar{V}_{11} \end{pmatrix} \mathcal{A},$$

for (3.26) to hold we need $V_{11} = -V_{22} =: W_1$. From (3.3) we see that W_1 is Λ -periodic and there exists Λ -periodic W_0 such that

$$\begin{pmatrix} 2D_{\bar{z}} + W_1 & 0 \\ 0 & 2D_{\bar{z}} - W_1 \end{pmatrix} = \begin{pmatrix} e^{W_0(z)} & 0 \\ 0 & e^{-W_0(z)} \end{pmatrix} \begin{pmatrix} 2D_{\bar{z}} & 0 \\ 0 & 2D_{\bar{z}} \end{pmatrix} \begin{pmatrix} e^{-W_0(z)} & 0 \\ 0 & e^{W_0(z)} \end{pmatrix}, \\ 2D_{\bar{z}}W_0 = W_1, \quad W_0(\omega z) = W_0(z).$$

(From (3.10) we see that $W_1(\omega z) = \omega W_1(z)$ and hence the integral of W_1 over \mathbb{C}/Λ is equal to 0; this shows that we can find W_0 , which is unique up to an additive constant.) We conclude that if we insist on (3.26) then we can, without loss of generality assume that

$$V(z) = \begin{pmatrix} 0 & V_{12}(z) \\ V_{21}(z) & 0 \end{pmatrix}, \quad (3.29)$$

$$V_{ij}(z + \gamma) = e^{i\langle k_j - k_i, \gamma \rangle} V_{ij}(z), \quad k_\ell \in \mathcal{K}, \quad k_1 \neq k_2, \quad V_{ij}(\omega z) = \omega V_{ij}(z).$$

To verify the latter we check that, with $w = (w_1, w_2)$,

$$\begin{aligned} \begin{pmatrix} 2D_{\bar{z}} & V_{12} \\ V_{21} & 2D_{\bar{z}} \end{pmatrix} \mathcal{A}w &= \begin{pmatrix} 2D_{\bar{z}}\Gamma w_2 - V_{12}\Gamma w_1 \\ -2D_{\bar{z}}\Gamma w_1 + V_{21}\Gamma w_2 \end{pmatrix} = \begin{pmatrix} \Gamma(-2D_z w_2 - \bar{V}_{12}w_1) \\ \Gamma(2D_z w_1 + \bar{V}_{21}w_2) \end{pmatrix} \\ &= - \begin{pmatrix} 0 & \Gamma \\ -\Gamma & 0 \end{pmatrix} \begin{pmatrix} 2D_z w_1 + \bar{V}_{21}w_2 \\ 2D_z w_2 + \bar{V}_{12}w_1 \end{pmatrix} = -\mathcal{A} \begin{pmatrix} 2D_{\bar{z}} & V_{12} \\ V_{21} & 2D_{\bar{z}} \end{pmatrix}^* w. \end{aligned}$$

Remarks. 1. The antilinear symmetry is closely related to the $C_{2z}T$ symmetry in the physics literature.

2. In the case when $V_{21}(z) = V_{12}(-z)$, we have another antilinear symmetry:

$$Qv(z) := -\mathcal{A}\mathcal{E}v(z) = \overline{v(-z)}, \quad QD(\alpha)Q = D(\alpha)^*. \quad (3.30)$$

The mapping property is simpler than (3.27): $Q : L_{k,p}^2(\mathbb{C}/\Lambda; \mathbb{C}^2) \rightarrow L_{k,-p}^2(\mathbb{C}/\Lambda; \mathbb{C}^2)$.

3.6. Theta functions. We now review properties of theta functions. To simplify notation we put $\theta(z) := \theta_1(z|\omega) := -\theta_{\frac{1}{2}, \frac{1}{2}}(z|\omega)$, and recall that

$$\theta(z) = - \sum_{n \in \mathbb{Z}} \exp(\pi i(n + \frac{1}{2})^2 \omega + 2\pi i(n + \frac{1}{2})(z + \frac{1}{2})), \quad \theta(-z) = -\theta(z) \quad (3.31)$$

$$\theta(z + m) = (-1)^m \theta(z), \quad \theta(z + n\omega) = (-1)^n e^{-\pi i n^2 \omega - 2\pi i z n} \theta(z),$$

and that θ has simple zeros at Λ (and no other zeros) – see [KhZa15].

We now define

$$F_k(z) = e^{\frac{i}{2}(z-\bar{z})k} \frac{\theta(z - z(k))}{\theta(z)}, \quad z(k) := \frac{\sqrt{3}k}{4\pi i}, \quad z : \Lambda^* \rightarrow \Lambda. \quad (3.32)$$

Then, using (3.31) and differentiating in the sense of distributions,

$$\begin{aligned} F_k(z + m + n\omega) &= e^{-nk \operatorname{Im} \omega} e^{2\pi i n z(k)} F_k(z) = F_k(z), \\ (2D_{\bar{z}} + k)F_k(z) &= c(k)\delta_{\Lambda}(z), \quad c(k) := 2\pi i \theta(z(k))/\theta'(0). \end{aligned} \quad (3.33)$$

(Here $\delta_{\Lambda}(z) := \sum_{\gamma \in \Lambda} \delta_0(z - \gamma)$ and we used the fact that if f and g are holomorphic, $g(\zeta)$ has a simple zero at 0 and $f(0) \neq 0$ then, near 0, $\partial_{\bar{\zeta}}(f(\zeta)/g(\zeta)) = \pi f(0)/g'(0)\delta_0(\zeta)$ – see for instance [Höl, (3.1.12)].)

The following Lemma is now immediate. It reinterprets the theta function argument in [TKV19].

Lemma 3.4. *Suppose that $p \in \mathcal{K}$ and $u \in \ker_{H_p^1}(D(\alpha) + k)$. Then*

$$(D(\alpha) + k + k')(F_{k'}(z - z(k''))u(z)) = c(k' - k'')\delta_{z(k'')}(z)u(z(k'')), \quad k, k', k'' \in \mathbb{C}, \quad (3.34)$$

where $c(k)$ is given in (3.33). In particular, if $u(z(k'')) = 0$ then

$$F_{k'}(z - z(k''))u(z) \in \ker_{H_p^1}(D(\alpha) + k + k'). \quad (3.35)$$

3.7. Multiplicity one. The definition of the set of *magic* α 's based on Proposition 3.3 does *not* involve the notion of multiplicity. Here we will discuss the case of multiplicity one[†]. One natural definition of multiplicity of magic angles is given in terms of eigenvalues of $H_k(\alpha)$ in (3.22). We first note that

$$\alpha \in \mathcal{A} \iff \forall k \in \mathbb{C}/\Lambda^*, \quad E_{\pm 1}(\alpha, k) = 0. \quad (3.36)$$

We then say, that the magic angle $\alpha \in \mathcal{A}$ is simple/has multiplicity one, if and only if

$$\forall k \in \mathbb{C}, \quad j > 1, \quad E_j(\alpha, k) > 0. \quad (3.37)$$

As stated in (2.9) we use a stronger definition in this paper.

The operators

$$\mathbb{C}^2 \ni (\alpha, k) \longmapsto D(\alpha) + k : H_0^1 \rightarrow L_0^2,$$

form a continuous family of Fredholm operators of index 0. (This follows from the ellipticity of $D(\alpha)$, the continuity of the index and then fact (3.36) implies that $D(\alpha) - k$ is invertible for some k and α .) In particular, $\dim \ker(D(\alpha) + k) = \dim \operatorname{coker}(D(\alpha)^* + \bar{k}) = \dim \ker(D(\alpha)^* - \bar{k})$, and hence

$$(3.37) \iff \forall k \in \mathbb{C}, \quad \dim \ker_{H_0^1}(D(\alpha) + k) = 1. \quad (3.38)$$

In [BHZ22b, Theorem 2] we proved that

Proposition 3.5. *Suppose (3.29) holds and that*

$$k_0 \in \mathcal{K} \setminus \{k_1, k_2\}, \quad k_1 \not\equiv k_2 \pmod{\Lambda^*}.$$

Then for $\alpha \in \mathcal{A}$ we have

$$(3.37) \iff \exists k \not\equiv k_1, k_2 \pmod{\Lambda^*}, \quad \dim \ker_{H_0^1}(D(\alpha) + k) = 1.$$

In particular, $\alpha \in \mathbb{C}$ is a simple magic angle (in the sense of (3.37)) if and only if

$$\dim \ker_{H_0^1}(D(\alpha) + k_0) = 1. \quad (3.39)$$

We recall that the proof is based on Proposition 3.3 and theta function arguments reviewed in §3.6.

A symmetric choice of ρ in (3.2) is given by:

$$k_1 = \frac{4\pi}{i\sqrt{3}}\left(\frac{1}{3} + \frac{2}{3}\omega\right) = \frac{4}{3}\pi =: K, \quad k_2 = -K = \frac{4}{3}\pi, \quad k_0 = 0. \quad (3.40)$$

This corresponds to $\Gamma = 0$ in the physics notation. In [Be*22] we followed [TKV19] and used a non-symmetric (equivalent) choice. This corresponds to the assumptions in (2.2) with $k_1 = K$.

[†]A more general discussion is presented in [BHZ23] – generic simplicity presented there is modified in view of protected multiplicity two magic angles – see the proof of Proposition 3.6.

Proposition 3.6. *Suppose that (3.39) holds. Then, in the notation of Lemma 3.1,*

$$\ker_{H_0^1}(D(\alpha) + k_0) = \mathbb{C}\tau(k_0)^*u_0, \quad \|u_0\|_{L_{k_0}^2} = 1, \quad \Omega u_0 = \omega u_0, \quad (3.41)$$

that is, in the notation of (3.20), $u_0 \in L_{k_0,2}^2$. In addition,

$$u_0(z) = zw(z), \quad w \in C^\infty(\mathbb{C}; \mathbb{C}^2), \quad w(0) \neq 0, \quad u_0(z) \neq 0, \quad z \notin \Lambda. \quad (3.42)$$

Remark. The key insight in [TKV19] was to use vanishing of $u \in \ker_{H_{k_1}^1} D(\alpha)$ for magic α 's at a distinguished point z_S to show that $\text{Spec}_{H_0^1}(D(\alpha)) = \mathbb{C}$. In [Be*22, Theorems 1] this was shown equivalent to the spectral definition based on Proposition 3.3. Here we take a direct approach: only at magic α 's we have $\ker_{H_{k_0}^1} D(\alpha) \neq \{0\}$ and (3.41) shows that its elements have to vanish at 0. Lemma 3.34 then implies vanishing of other eigenfunctions.

Proof of Proposition 3.6. From Lemma 3.1 and (3.39) we conclude that $\ker_{H_{k_0}^1} D(\alpha) = \mathbb{C}u_0$ and as $L_{k_0}^2 = \bigoplus_{j=0}^2 L_{k_0,j}^2$ we can decompose the kernel using these subspaces. Since $D(0) + k_0 : H_0^1 \rightarrow L_0^2$ is invertible (see (3.9)), (3.19) shows that $D(0) : H_{k_0}^1 \rightarrow L_{k_0}^2$ is invertible with the inverse given by $R(0)$. It then follows that (see (3.25))

$$I + \alpha T_0 = R(0)D(\alpha) : L_{k_0,j}^2 \rightarrow L_{k_0,j}^2, \quad \ker_{H_{k_0}^1} D(\alpha) = \ker_{L_{k_0,j}^2} R(0)D(\alpha).$$

(We do use ellipticity of $D(\alpha)$ here: the element of the kernel on L^2 must automatically be smooth.) Hence if $\ker_{L_{k_0,j}^2} (R(0)D(\alpha)) \neq \{0\}$, $j = 0, 1$, then $\ker_{L_{k_0,j}^2} (D(\alpha)^*R(0)^*) \neq \{0\}$, and there exists $w \in L_{k_0,j}^2$ such that $D(\alpha)^*R(0)^*w = 0$. We now note that

$$R(0)^* : L_{k_0,j}^2 \rightarrow L_{k_0,j-1}^2. \quad (3.43)$$

In fact, $2D_{\bar{z}} = D(0) : H_{k_0}^1 \rightarrow L_{k_0}^2$ is invertible by Proposition 3.2 and 3.3 and $R(0) : L_{k_0}^2 \rightarrow H_{k_0}^1 \subset L_{k_0}^2$ is its inverse. Since $2D_{\bar{z}}[u(\omega^\ell z)] = (\bar{\omega})^\ell [2D_{\bar{z}}u](\omega^\ell z)$, if $u(\omega^\ell z) = \bar{\omega}^{\ell p}$ then $[2D_{\bar{z}}u](\omega^\ell z) = \bar{\omega}^{\ell(p-1)}$. Hence, in terms of definition (3.20), $2D_{\bar{z}} : H_{k_0,j}^1 \rightarrow L_{k_0,j-1}^2$. Consequently, $R(0) : L_{k_0,j-1}^2 \rightarrow L_{k_0,j}^2$ and as the dual space to $L_{k_0,p}^2$ (using the L^2 pairing) is given by $L_{k_0,p}^2$, (3.43) follows.

This and $\mathcal{A} : L_{k_0,j-1}^2 \rightarrow L_{k_0,-j+1}^2$ (see (3.28)) show

$$D(\alpha)\mathcal{A}R(0)^*w = 0, \quad \mathcal{A}R(0)^*w \in L_{k_0,-j+1}^2 \neq L_{k_0,j}^2 \quad \text{when } j = 0, 1.$$

This means that $\dim \ker_{H_{k_0}^1} D(\alpha) > 1$, contradicting the simplicity assumption. The simplicity and uniqueness of the zero of u_0 (3.42) follows from [BHZ22b, Theorem 3]. \square

For an $\alpha \in \mathcal{A}$, we assume that (3.39) holds. In that case Proposition 3.6 and Lemma 3.4 show that

$$\ker_{H_0^1}(D(\alpha) + k) = \mathbb{C}u(k), \quad u(k) := \frac{F_k u_0}{\|F_k u_0\|}. \quad (3.44)$$

Using (3.26) we see that (since $\mathcal{A}^2 = -I$)

$$(D(\alpha)^* + \bar{k})\mathcal{A} = -\mathcal{A}(D(\alpha) - k),$$

which implies that

$$\ker_{H_0^1}(D(\alpha)^* + \bar{k}) = \mathbb{C}\mathcal{A}u(-k). \quad (3.45)$$

Remark. From [BHZ22b, (6.6)] we see that (note the difference of notation: $u(k)$ there is not normalized) for the basis of Λ^* satisfying $z(e_1) = 1$, $z(e_2) = \omega$, we have for $p = me_1 + ne_2 \in \Lambda^*$,

$$u(k+p) = e_p(k)^{-1}\tau(p)u(k), \quad e_p(k) := e^{-\frac{1}{2}\pi in^2 + \pi i(k+\bar{k})n}(-1)^{n+m}, \quad (3.46)$$

where the unitary operator $\tau(p)$ was defined in (3.7).

4. GRUSHIN PROBLEMS

In this section we construct Grushin problems (see [SjZw07] and [DyZw19, §C.1]) which allow us to treat small in-plane magnetic fields as perturbations. In §5 we combine that with the spectral characterization of magic angles (Proposition 3.3) to analyze the behaviour at the Γ point and at the vertices of the boundary of the Brillouin zone.

4.1. **Grushin problem for $D_B(\alpha)$.** Suppose $\underline{\alpha} \in \mathcal{A}$ is simple, in the sense that (3.39) holds. We then put, in the notation of (3.44) and (3.45),

$$\begin{aligned} \mathcal{D}_B(\underline{\alpha}, k) &= \begin{pmatrix} D(\underline{\alpha}) + k & R_-(k) \\ R_+(k) & 0 \end{pmatrix} + \begin{pmatrix} \sigma_3 B & 0 \\ 0 & 0 \end{pmatrix} : H_0^1 \times \mathbb{C} \rightarrow L_0^2 \times \mathbb{C}, \\ R_-(k)u_- &= u^*(k)u_-, \quad R_+(k)u = \langle u, u(k) \rangle, \\ (D(\underline{\alpha}) + k)u(k) &= 0, \quad \|u(k)\| = 1, \quad u^*(k) = \mathcal{A}u(-k). \end{aligned} \quad (4.1)$$

We have

$$\mathcal{D}_B(\underline{\alpha}, k)^{-1} = \begin{pmatrix} E^B(k) & E_+^B(k) \\ E_-^B(k) & E_-^B(k) \end{pmatrix},$$

where

$$\begin{aligned} E_+^0 v_+ &:= u(k)v_+, \quad E_-^0 v := \langle v, u^*(k) \rangle, \quad E_{-+}^0 = 0, \\ E^0 v &:= ((D(\underline{\alpha}) + k)|_{(\mathbb{C}u(k))^\perp \rightarrow (\mathbb{C}u^*(k))^\perp})^{-1} (v - \langle v, u^*(k) \rangle u^*(k)). \end{aligned} \quad (4.2)$$

We now apply [DyZw19, Lemma C.3] to obtain

$$\begin{aligned} E_{-+}^B &= -E_- \sigma_3 B E_+ + \mathcal{O}(B^2) = -c(k)c^*(k)B(G(k) + \mathcal{O}(B)), \\ G(k) &:= (c(k)c^*(k))^{-1} (\langle u_1(k), u_1^*(k) \rangle - \langle u_2(k), u_2^*(k) \rangle), \end{aligned} \quad (4.3)$$

and, if $u_0 = (\psi, \varphi)^t$, and $u(k) = (u_1(k), u_2(k))^t$ then

$$u_1(k) = c(k)F_k\psi, \quad u_2(k) = c(k)F_k\varphi, \quad u_1^*(k) = c^*(k)\overline{F_{-k}\varphi}, \quad u_2^* = -c^*(k)\overline{F_{-k}\psi},$$

where $c(k), c^*(k) > 0$ come from L^2 -normalizations of u and u^* .

Hence,

$$G(k) = 2 \int_{\mathbb{C}/\Lambda} F_k(z) F_{-k}(z) \varphi(z) \psi(z) dm(z).$$

In fact $G(k)$ is a multiple of $\theta(z(k))^2$ which follows from a theta function identity (see [KhZa15, (4.7a)])

$$\theta(z+u)\theta(z-u)\theta_2(0)^2 = \theta^2(z)\theta_2^2(u) - \theta_2^2(z)\theta^2(u), \quad \theta_2(z) := \theta(z + \frac{1}{2}). \quad (4.4)$$

Since, (from $u \in H_{0,2}^1$)

$$\int_{\mathbb{C}/\Lambda} \varphi(z)\psi(z)dm(z) = \int_{\mathbb{C}/\Lambda} \varphi(\omega z)\psi(\omega z)dm(z) = \omega^2 \int_{\mathbb{C}/\Lambda} \varphi(z)\psi(z)dm(z),$$

this integral vanishes, and (4.4) gives

$$G(k) = g_0 \frac{\theta(z(k))^2}{\theta(\frac{1}{2})^2}, \quad g_0 = g_0(\underline{\alpha}) := 2 \int_{\mathbb{C}/\Lambda} \theta(z + \frac{1}{2})^2 \frac{\varphi(z)\psi(z)}{\theta(z)^2} dm(z). \quad (4.5)$$

Numerical evidence, see Table 1, suggests that for the Bistritzer–MacDonald potential and the first magic angle,

$$|g_0| \simeq 0.07 \neq 0.$$

(The number g_0 is determined up to phase which we can choose arbitrarily by modifying $u_0 \mapsto e^{i\theta}u_0$.) Table 1 shows approximate values of $|g_0|$ for higher magic angles for the same potential.

Remark. We also see that the Grushin problem (4.1) remains well posed with $\underline{\alpha}$ replaced with α , $|\underline{\alpha} - \alpha| \ll 1$. The effective Hamiltonian (4.3) has to be modified by term (obtained again using [SjZw07, Proposition 2.12])

$$\begin{aligned} E_{-+}^B(k, \alpha) &= E_{-+}^B(k) - (\alpha - \bar{\alpha})f_2(k, B, \alpha), \\ f_2(k, 0, \underline{\alpha}) &:= g_1(k, \underline{\alpha}) = -E_-^0(k) \begin{pmatrix} 0 & U(z) \\ U(-z) & 0 \end{pmatrix} E_+^0(k), \end{aligned} \quad (4.6)$$

where and in the notation following (4.3),

$$\begin{aligned} g_1(k, \underline{\alpha}) &:= \int_{\mathbb{C}/\Lambda} (U(-z)u_1(k, z)u_1(-k, z) - U(z)u_2(k, z)u_2(-k, z))dm(z) \\ &= \int_{\mathbb{C}/\Lambda} F_k(z)F_{-k}(z)(U(-z)\psi(z)^2 - U(z)\varphi(-z)^2)dm(z). \end{aligned} \quad (4.7)$$

An indirect argument presented in the proof of Proposition 5.1 shows that if $g_0(\underline{\alpha}) \neq 0$ then $g_1(0, \underline{\alpha}) \neq 0$. This can also be verified numerically – see Table 1.

4.2. Grushin problem for the self-adjoint Hamiltonian. We now turn to the corresponding Grushin problem for $H_k^B(\alpha)$ given in (3.5) (note the irrelevant change of sign of k)

$$\begin{aligned} \mathcal{H}_k^B(\alpha, z) &:= \begin{pmatrix} H_k^B(\alpha) - z & \tilde{R}_-(k) \\ \tilde{R}_+(k) & 0 \end{pmatrix} : H_0^1(\mathbb{C}/\Lambda; \mathbb{C}^4) \times \mathbb{C}^2 \rightarrow L_0^2(\mathbb{C}/\Lambda; \mathbb{C}^4) \times \mathbb{C}^2, \\ H_k^B(\alpha) &:= \begin{pmatrix} 0 & D_B(\alpha)^* + \bar{k} \\ D_B(\alpha) + k & 0 \end{pmatrix}, \\ \tilde{R}_-(k) &= \begin{pmatrix} 0 & R_+(k)^* \\ R_-(k) & 0 \end{pmatrix}, \quad \tilde{R}_+(k) = \tilde{R}_-(k)^*, \end{aligned} \tag{4.8}$$

where $R_\pm(k)$ are the same as in (4.1). The operator $\mathcal{H}_k^B(\alpha, z)$ is invertible for all k , $|B| \ll 1$, $|\alpha - \underline{\alpha}| \ll 1$ and $|z| \ll 1$. We denote the components of the inverse by $\tilde{E}_\bullet^B(k, \alpha, z)$ and we have

$$\tilde{E}_+^0(k, \underline{\alpha}, 0) = \begin{pmatrix} 0 & E_+^0(k) \\ E_-^0(k)^* & 0 \end{pmatrix}, \quad \tilde{E}_-^0(k, \underline{\alpha}, 0) = \tilde{E}_+^0(k, \underline{\alpha}, 0)^*, \quad \tilde{E}_{-+}^0(k, \underline{\alpha}, 0) \equiv 0.$$

Using [DyZw19, Lemma C.3] again we see that (in the notation of (4.6))

$$\tilde{E}_{-+}^B(k, \alpha, z) = \begin{pmatrix} z & E_{-+}^B(k, \alpha) \\ E_{-+}^B(k, \alpha)^* & z \end{pmatrix} + \mathcal{O}(|z|^2 + |B|^2 + |\alpha - \underline{\alpha}|^2).$$

(Here we used the fact that $E_-^0(k)E_-^0(k)^* \equiv 1$ and $E_+^0(k)^*E_+^0(k) \equiv 1$ which follows from (4.2) and normalization of $u(k)$ and $u^*(k)$.)

Hence $z = E_1^B(k, \alpha) = -E_{-1}^B(k, B)$ (the eigenvalues of $H_k^B(\alpha)$ closest 0) for k close to 0 are given by solutions of

$$\begin{aligned} \det \tilde{E}_\pm^B(k, \alpha, z) = 0 &\implies \\ z &= \pm |\gamma_1 B k^2 + \gamma_0(\alpha - \underline{\alpha}) + \mathcal{O}(|B|^2 + |\alpha - \underline{\alpha}|^2 + |k|^4)|, \end{aligned} \tag{4.9}$$

where (under the assumption that $g_0(\underline{\alpha}) \neq 0$) $\gamma_0 \neq 0$, $\gamma_1 \neq 0$. (The exact symmetry of signs follows from the extension of the chiral symmetry (3.16) to the Grushin problem (4.8) which shows that $\det \tilde{E}_\pm^B(k, \alpha, z) = \det \tilde{E}_\pm^B(k, \alpha, -z)$.)

5. BIFURCATION

This section is devoted to showing (2.18) and giving a stronger version of Theorem 3.

We first observe that for $\pm B - k \notin \mathcal{K}_0 = \{K, -K\} + \Lambda^*$, $K = \frac{4}{3}\pi > 0$,

$$((2D_{\bar{z}} - k)I_{\mathbb{C}^2} + \sigma_3 B)^{-1} : L_0^2 \rightarrow H_0^1,$$

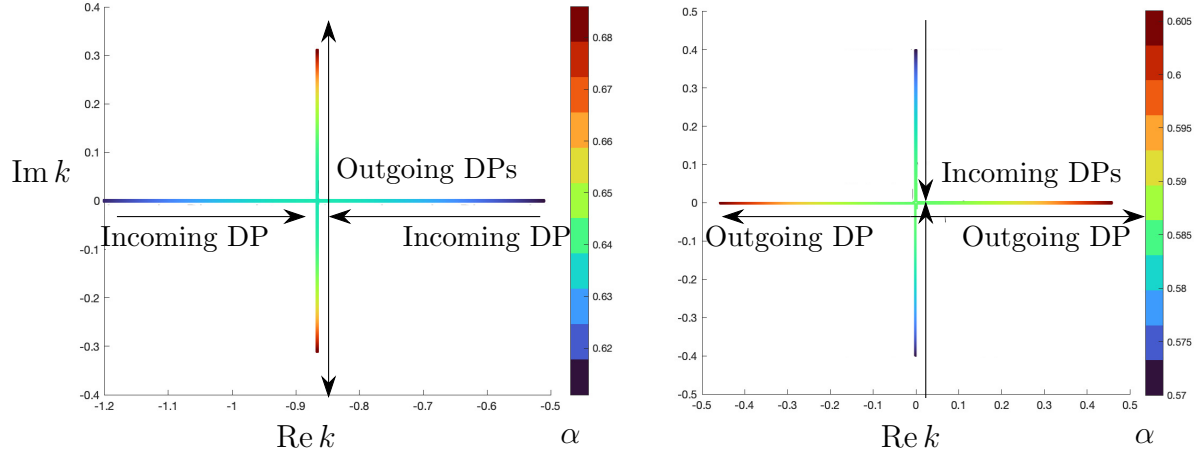


FIGURE 6. Bifurcation for $B = 0.1$. (Top): The color-coding indicates the position of the Dirac points for given values of $\alpha \in \mathbb{R}$. The right figure illustrates the bifurcation at Γ and the left figure at a non-equivalent (modulo Λ^*) bifurcation point that is a vertex of the boundary of the Brillouin zone, see Figure 1.

and we can define

$$T_k(B) := ((2D_{\bar{z}} - k)I_{\mathbb{C}^2} + \sigma_3 B)^{-1} \begin{pmatrix} 0 & U(z) \\ U(-z) & 0 \end{pmatrix}. \quad (5.1)$$

It then follows that for $\pm B - k \notin \mathcal{K}_0 = \{K, -K\} + \Lambda^*$,

$$k \in \text{Spec}_{L_0^2}(D_B(\alpha)) \iff 1/\alpha \in \text{Spec}_{L_0^2}(T_k(B)). \quad (5.2)$$

In particular, this characterization holds when $k \in \mathbb{C} \setminus (\mathcal{K}_0 + D(0, \delta))$ and $|B| < \frac{1}{2}\delta$. However, in Figure 8 we will show and discuss the spectrum of $T_k(B)$ when $k \in \mathcal{K}_0$ and $B \neq 0$.

Combining the spectral characterization with the result of §4 we can obtain a rather precise characterization of the behaviour of eigenvalues of $T_k(B)$:

Proposition 5.1. *Suppose that $\underline{\lambda}$ is a simple eigenvalue of $T_k = T_k(0)$ and that assumptions of Theorem 2 hold for $\underline{\alpha} = 1/\underline{\lambda}$. Then for every $\varepsilon > 0$ there exists $\delta > 0$ and a holomorphic function $\lambda(k, B)$, such that $\lambda(k, B)$ is a simple eigenvalue of $T_k(B)$ and*

$$\begin{aligned} (k, B) &\mapsto \lambda(k, B), \quad k \in \Omega_\varepsilon := \mathbb{C} \setminus (\mathcal{K}_0 + D(0, \varepsilon)), \quad B \in D(0, \delta) \\ \lambda(k + p, B) &= \lambda(k, B), \quad p \in \Lambda^*, \quad k, k + p \in \Omega_\varepsilon, \quad B \in D(0, \delta), \\ \lambda(k, B) &= -\overline{\lambda(\bar{k}, \bar{B})} = \lambda(\omega k, \omega B) = \lambda(-k, B), \\ \lambda(k, 0) &= \underline{\lambda}, \quad \partial_B \partial_k^2 \lambda(0, 0) \in \mathbb{R} \setminus \{0\}. \end{aligned} \quad (5.3)$$

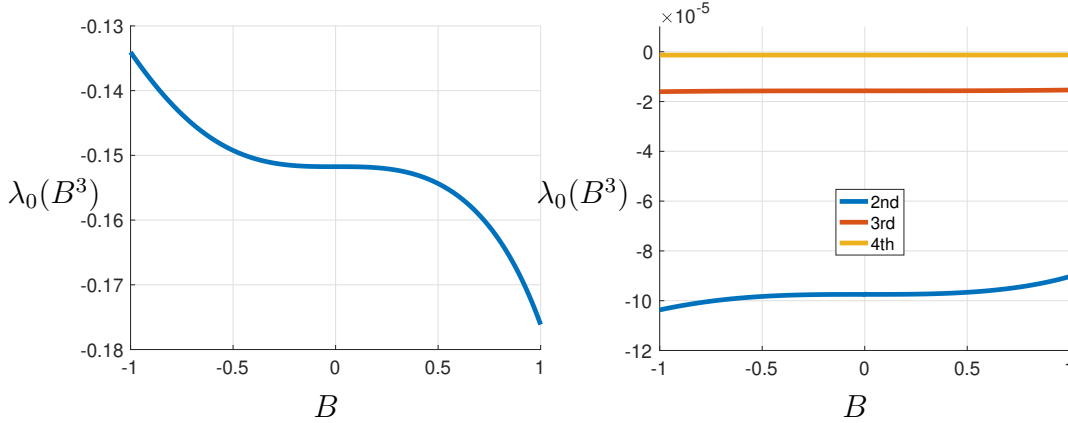


FIGURE 7. Plot of the $B \mapsto \lambda_1(B)$ of Proposition 5.1 for the first (left) and second to fourth magic angle (right).

In particular, for $B \in D(0, \delta) \subset \mathbb{C}$,

$$\lambda(k, B) = \underline{\lambda} + c_1 B k^2 + \lambda_1(B^3) B^3 + \mathcal{O}(B^4 k^2) + \mathcal{O}(B^2 k^4) + \mathcal{O}(B k^8), \quad (5.4)$$

where $c_1 \in \mathbb{R} \setminus \{0\}$, $\lambda_1(z) = \bar{\lambda}_1(\bar{z})$,

Remarks. 1. It follows from the proof that the constant c_1 can be computed using the constants $g_0(\underline{\alpha})$ and $g_1(\underline{\alpha})$ defined in (4.5) and (4.6) respectively:

$$c_1 = -\frac{3\theta'(0)^2}{16\pi^2\theta(\frac{1}{2})^2} \frac{g_0(\underline{\alpha})}{g_1(\underline{\alpha})}.$$

2. In view of (5.2), (5.4), shows that when $\underline{\alpha}$ is magical and $\underline{\lambda} = 1/\underline{\alpha}$ satisfies the assumptions of Proposition 5.1, then for $0 < |B| \ll 1$, $k \in \text{Spec}_{L_0^2} D_B(\alpha) \cap D(0, \delta)$, $0 < \delta \ll 1$, if and only if

$$Bk^2(1 + \mathcal{O}(k^8)) = c_1^{-1}(1 - \alpha/\underline{\alpha}) + \mathcal{O}(B^3). \quad (5.5)$$

In particular, when B and α are real then the eigenvalues of $D_B(\alpha)$ bifurcate $k = 0$ when α is chosen so that the right hand side of (5.5) vanishes. (We recall from (5.4) that $c_1 \in \mathbb{R} \setminus \{0\}$ and $\lambda_1(B^3)$ is real for B real). We see the same bifurcation for $B = B_0 e^{\pm 2\pi i/3}$, $B_0 > 0$, obtained using (2.10).

3. Numerical evidence suggests (see Figure 7) that $\partial_B^3 \lambda(0, 0) < 0$ for the Bistritzer-MacDonald potential. If $B = B_0 e^{2\pi i\theta}$ that means the Γ point (corresponding $k = 0$) is in the spectrum of $D_B(\alpha)$, $\alpha \in \mathbb{R}$, only if $\theta \in \frac{1}{3}\mathbb{Z}$.

Proof of Proposition 5.1. Let $U \Subset \mathbb{C} \setminus \mathcal{K}_0$ be an open set. Then for $k \in U$, $T_k(B) = T_k(0) + \mathcal{O}(B)_{L_0^2 \rightarrow L_0^2}$ and if $0 < \varepsilon_0 \ll 1$, then the projection, $\Pi(k, B) := (2\pi i)^{-1} \int_{\partial D(\underline{\lambda}, \varepsilon_0)} (\zeta - T_k(B))^{-1} d\zeta$, is holomorphic in k and B and has a fixed rank. We assumed that

$T_k(0)$ has a simple eigenvalue at $\underline{\lambda}$ (independent of k – see (3.24)), which then implies that the rank is one, and $T_k(B)$ has a simple eigenvalue $\lambda = \lambda(k, B)$. Since $\lambda(k, B) = \text{tr}(T_k(B)\Pi(k, B))$ it follows that $\lambda(k, B)$ is holomorphic in k and B .

From (2.10) and (5.1) we conclude that

$$\text{Spec}_{L_0^2}(T_k(B)) = \overline{\text{Spec}_{L_0^2}(T_{\bar{k}}(\bar{B}))} = \text{Spec}_{L_0^2}(T_{-k}(B)) = \text{Spec}_{L_0^2}(T_{\omega k}(\omega B)), \quad (5.6)$$

This gives

$$\lambda(k, B) = \lambda(-k, B) = \overline{\lambda(\bar{k}, \bar{B})} = \lambda(\omega k, \omega B). \quad (5.7)$$

Definitions (5.2) and (3.7) give $T_{k+p}(B) = \tau(p)T_k(B)\tau(p)^*$, $p \in \Lambda^*$, and hence

$$\lambda(k+p, B) = \lambda(k, B), \quad p \in \Lambda^* \quad (5.8)$$

provided that $k, k+p \in U$. This allows an extension of $\lambda(k, B)$ to Ω_ε in the statement of the proposition, provided that $|B| < \delta$ for some sufficiently small δ . The properties of the expansion (5.4) come from the fact that individual terms in the Taylor expansion satisfy the symmetries (5.7):

$$\begin{aligned} a_{pq}k^p B^q = a_{pq}(-1)^p k^p B^q = \bar{a}_{pq}k^p B^q = a_{pq}\omega^{p+q}k^p B^q, \quad a_{pq} \neq 0 \implies \\ a_{pq} \in \mathbb{R}, \quad p = 2\ell, \quad \ell \in \mathbb{N}, \quad q \equiv \ell \pmod{3}. \end{aligned} \quad (5.9)$$

This proves (5.3) and (5.4) except for $c_1 \neq 0$, that is, the non-vanishing of $\partial_B \partial_k^2 \lambda(0, 0)$.

To establish that, we compare the expansion of $\lambda(k, B)$ with the effective Hamiltonian (4.6):

$$\lambda(k, B) = \lambda \iff E_{-+}^B(k, \alpha) = 0, \quad \alpha = \lambda^{-1}.$$

We now define μ by

$$\lambda = \underline{\lambda}(1 - \mu\underline{\lambda}), \quad \lambda^{-1} = \underline{\lambda}^{-1}(1 - \underline{\lambda}\mu)^{-1} = \underline{\lambda}^{-1} + \mu + \mathcal{O}(\mu^2).$$

Using (4.6) and (4.3), $E_{-+}^B(k, \alpha) = 0$ becomes

$$Bk^2 + a_0^{-1}\mu g_1(k, \underline{\alpha}) + \mathcal{O}(\mu^2) + \mathcal{O}(B^2) + \mathcal{O}(Bk^3) = 0, \quad (5.10)$$

$a_0 := -\underline{\alpha}g_0(\underline{\alpha})\theta(\frac{1}{2})^{-2}(\theta'(0))^2 \neq 0$, which is then equivalent to (5.4):

$$-\mu = \tilde{c}_1 b k^2 + \mathcal{O}(B^3) + \mathcal{O}(Bk^8), \quad \tilde{c}_1 := \underline{\lambda}^{-2}c_1. \quad (5.11)$$

Inserting (5.11) into (5.10) gives

$$Bk^2 = a_0^{-1}g_1(k, \underline{\alpha})\tilde{c}_1 Bk^2 + \mathcal{O}(B^2) + \mathcal{O}(Bk^3),$$

which should hold for (k, B) near $(0, 0)$ (since $\mu = \mu(k, B) = \underline{\lambda}^{-1} - \underline{\lambda}^{-2}\lambda(k, B)$). But that is possible only when $g_1(0, \underline{\alpha})\tilde{c}_1 \neq 0$ (we used here the numerically established assumption that $g_0(\underline{\alpha}) \neq 0$). Hence $\partial_B \partial_k^2 \lambda(0, 0) = \frac{1}{2}c_1 = \frac{1}{2}\underline{\lambda}^2 \tilde{c}_1 \neq 0$ and, as promised after (4.6), $g_1(0, \underline{\alpha}) \neq 0$. \square

At the bifurcation point, the Bloch eigenvalues exhibit a quadratic well, see Figure 3.

Proposition 5.2. *Under the assumptions, and in the notation, of Proposition 5.1 and (5.5), let α^* be the solution to*

$$\alpha^* = \underline{\alpha} + \underline{\alpha}^2(B)^3 \lambda_1(B^3),$$

so that $0 \in \text{Spec}_{L_0^2} D_B(\alpha^*)$. Then the two Bloch eigenvalues $E_{\pm 1}$ of $H_k^B(\alpha)$ closest to zero, defined in (3.22), satisfy

$$E_{\pm 1}(\alpha^*, k) = \pm |\gamma_1 B k^2| + \mathcal{O}(B^2 + |k|^4), \quad \gamma_1 > 0.$$

Proof. This follows from (4.9) and (5.5). \square

The next proposition deals with the vertices of the boundary of the Brillouin zone. In view of (5.8) it is enough to consider one of the vertices, say,

$$\underline{k}_1 := 2\pi i / \sqrt{3}, \quad z(\underline{k}_1) = \frac{1}{2}. \quad (5.12)$$

We will crucially use the following properties of the theta function defined in (3.31):

$$\theta(\frac{1}{2}) \neq 0, \quad \theta'(\frac{1}{2}) = 0, \quad \theta''(\frac{1}{2}) \neq 0. \quad (5.13)$$

The first property follows from the fact that the only zeros of θ lie on Λ . The second one comes from $\theta(-z) = -\theta(z)$ and $\theta(z+1) = -\theta(z)$ so that $w \mapsto \theta(\frac{1}{2} + w)$ is an even function. The last claim can be obtained from taking logarithmic derivatives of [KhZa15, (2.10b)] or by a rigorous numerical verification based on fast convergence of the sum in (3.31).

Proposition 5.3. *Suppose that $\underline{\lambda}$ is a simple eigenvalue of $T_k = T_k(0)$ and that assumptions of Theorem 2 hold for $\underline{\alpha} = 1/\underline{\lambda}$. Then, for k near \underline{k}_1 given in (5.12),*

$$\lambda(k, B) = \underline{\lambda} + B\lambda_2(B) + c_2 B(k - \underline{k}_1)^2 + \mathcal{O}(|B|^2 |k - \underline{k}_1|^2). \quad (5.14)$$

where $c_2, \lambda_2(0) \in \mathbb{R} \setminus \{0\}$.

Remark. We again have a bifurcation result similar to (5.5) but less precise:

$$B(k - \underline{k}_1)^2(1 + \mathcal{O}(B)) = c_2^{-1}(1 - \alpha/\underline{\alpha}) - B\lambda_2(\alpha^{-1}B) + \mathcal{O}(B^2). \quad (5.15)$$

For B real we see a bifurcation at $\alpha_* = \underline{\alpha} + B\lambda_2(B)$, with similar bifurcations for $B = B_0 e^{\pm 2\pi i/3}$, $B_0 > 0$, obtained using (2.10).

Proof of Proposition 5.3. From (5.7), (5.8) and the fact that $2k_1 = 4\pi i / \sqrt{3} \in \Lambda^*$ we conclude that

$$\begin{aligned} \lambda(\underline{k}_1 + z, B) &= \lambda(-\underline{k}_1 - z, B) = \lambda(\underline{k}_1 - z, B) \\ &= \overline{\lambda(-\bar{z} - \underline{k}_1, \bar{B})} = \overline{\lambda(\underline{k}_1 - \bar{z}, \bar{B})}. \end{aligned} \quad (5.16)$$

We also note that for $k \notin \mathcal{K}_0 + D(0, \varepsilon)$, $\lambda(k, 0) = \underline{\lambda}$ (since $k \in \text{Spec}_{L_0^2} D_0(\alpha)$ only at $\alpha = \underline{\alpha} = 1/\underline{\lambda}$). Hence, as in (5.11) and with the same definition of μ ,

$$-\mu = B\lambda_2(B) + \tilde{c}_2 B w^2 + \mathcal{O}(B^2 w^2), \quad w := \underline{k}_1 - k \quad \tilde{c}_2 := \underline{\lambda}^{-2} c_2, \quad \lambda_2(0) \in \mathbb{R}. \quad (5.17)$$

We now proceed as in the proof of Proposition 5.1 and use (4.6) and (5.13):

$$(\theta(z(k)))^2 = \theta(\tfrac{1}{2})^2 + \theta''(\tfrac{1}{2})w^2 + \mathcal{O}(w^4).$$

This gives the following equation:

$$a_1B + a_2Bw^2 + a_3\mu + \mathcal{O}(\mu^2) + \mathcal{O}(B^2) + \mathcal{O}(Bw^4) = 0, \quad a_1a_2 \neq 0. \quad (5.18)$$

Substituting (5.17) into (5.18) shows that $a_3 \neq 0$ and $c_2 \neq 0$. \square

6. PROOFS OF THEOREMS 2 AND 3

Combining the results of previous of sections we can now prove the main results of this paper.

Proof of Theorem 2. In the notation of (4.6) we see the effective Hamiltonian for $D_B(\underline{\alpha})$ for B small

$$E_{-+}^B(k, \alpha) = -Bc(k)c^*(k)(c_0\theta(z(k))^2 + \mathcal{O}(B)) + \mathcal{O}(\alpha - \underline{\alpha}). \quad (6.1)$$

Since $\theta(z(k)) \neq 0$ for $k \notin \Lambda^*$ (see §3.6) there exists a constant a_1 such that if $|\alpha - \underline{\alpha}| < a_1|B|$ then $E_{-+}^B(k)$ is not identically 0 (provided that B is small enough). This shows invertibility at some k and hence discreteness of the spectrum (by the analytic Fredholm theory applied to $k \mapsto (D_B(\alpha) - k)^{-1}$ – see for instance [DyZw19, Theorem C.8]) for

$$(B, \alpha) \in \Omega_1 := \{(B, \alpha) : |B| < \delta_1, \quad |\alpha - \underline{\alpha}| < a_1|B|\}. \quad (6.2)$$

On the other hand, we can put $k = 0$ and recall from the proof of Proposition 5.1 (see (4.6)) that

$$E_{-+}^B(0, \alpha) = c_0(\alpha - \underline{\alpha})(1 + \mathcal{O}(\alpha - \underline{\alpha}) + \mathcal{O}(B)) + \mathcal{O}(B^2), \quad c_0 \neq 0.$$

Hence $E_{-+}^B(0, \alpha)$ does not vanish if, for some constant A_1 , and small $\delta_2 > 0$,

$$(B, \alpha) \in \Omega_2 := \{(B, \alpha) : A_1|B|^2 < |\alpha - \underline{\alpha}| < \delta_2\}. \quad (6.3)$$

Again, that implies discreteness of the spectrum. We now note that there exists $\delta_0 > 0$ such that

$$(D(0, \delta_0) \setminus \{0\}) \times D(\underline{\alpha}, \delta_0) \subset \Omega_1 \cup \Omega_2,$$

and this proves discreteness of the spectrum of $D_B(\alpha)$ for $0 < |B| < \delta_0$ and $|\alpha - \underline{\alpha}| < \delta_0$.

We also see that (6.1) implies (2.16): for $U \Subset \mathbb{C}$, for any epsilon there exists $\rho > 0$ such that $|\theta(z(k))^2| > \rho$ for $z \in \mathcal{U} \setminus (\Lambda^* + D(0, \varepsilon))$. But then

$$|E_{-+}^B(k, \alpha)| > c_0c(k)c^*(k)|B|\rho - \mathcal{O}(B^2) - \mathcal{O}(|\alpha - \underline{\alpha}|) > 0,$$

if $0 < |B| \leq \rho/C$ and $|\alpha - \underline{\alpha}| < \rho|B|/C$ for some (large) constant C .

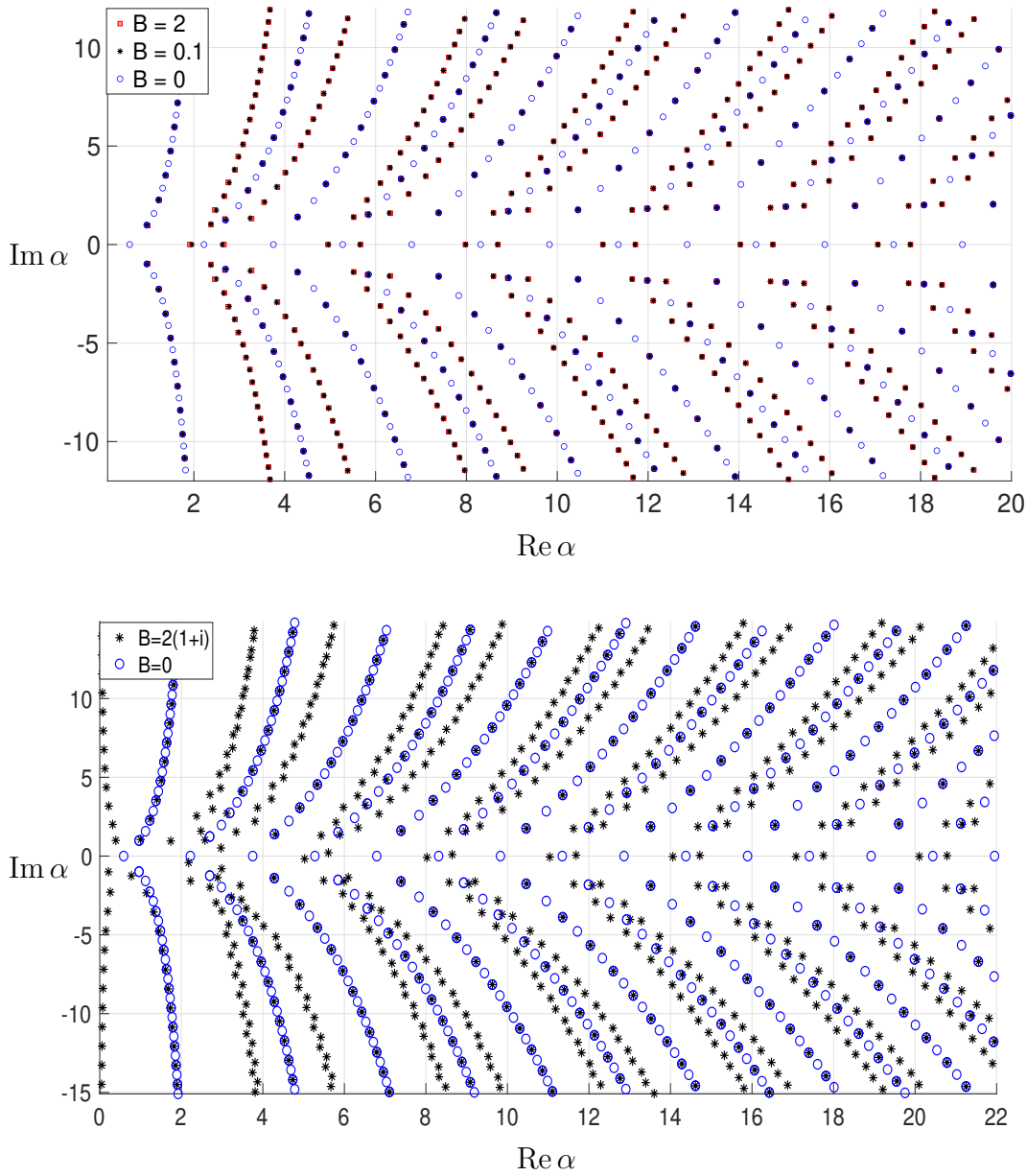


FIGURE 8. Top figure showing $\alpha \in \mathbb{C}$ such that $1/\alpha \in \text{Spec}_{L_0^2}(T_K(B))$ or $K \in \text{Spec}_{L_0^2}(D_B(\alpha))$. We see that indeed for $B \in \mathbb{R} \setminus \{0\}$ the trajectory of Dirac points passes through K, K' . Bottom figure showing $\alpha \in \mathbb{C}$ such that $1/\alpha \in \text{Spec}_{L_0^2}(T_K(B))$ or $K \in \text{Spec}_{L_0^2}(D_B(\alpha))$. For general $B \notin \mathbb{R}$ the trajectory of Dirac points for varying $\alpha \in \mathbb{R}$ does not pass through K between successive real magic angles.

It remains to prove (2.15). Let F be a fundamental domain of Λ^* containing 0 and such that there are no eigenvalues on ∂F (that can be arranged as under our assumptions the spectrum of $D_B(\alpha)$ is discrete and periodic with respect to Λ^*). Then,

$$|\text{Spec}_{L_0^2}(D_B(\alpha)) \cap F| = \frac{1}{2\pi i} \text{tr} \int_{\partial F} (\zeta - D_B(\alpha))^{-1} d\zeta.$$

As long $D_B(\alpha)$ has no eigenvalue on ∂F for $(B, \alpha) \in K \subset \mathbb{C}^2$, this value remains constant for $(B, \alpha) \in K$. Choosing a small ε and δ needed for (2.16) and putting $K = \{(B, \alpha) : |B| < \delta, |\alpha - \underline{\alpha}| < a_0 \delta |B|\}$, we see that (using [SjZw07, Proposition 4.2])

$$\begin{aligned} \frac{1}{2\pi i} \text{tr} \int_{\partial F} (\zeta - D_B(\alpha))^{-1} d\zeta &= \frac{1}{2\pi i} \text{tr} \int_{\partial D(0, \varepsilon)} (\zeta - D_B(\underline{\alpha}))^{-1} d\zeta \\ &= \frac{1}{2\pi i} \int_{\partial D(0, \varepsilon)} E_{-+}^B(\zeta)^{-1} d_\zeta E_{-+}^B(\zeta) \\ &= \frac{1}{2\pi i} \int_{\partial D(0, \varepsilon)} (\zeta^2 + \mathcal{O}(B))^{-1} (2\zeta + \mathcal{O}(B)) d\zeta \\ &= 2 + \mathcal{O}(B) = 2, \end{aligned}$$

provided B is small enough (depending on ε , note that $\alpha = \underline{\alpha}$ in the calculation; the answer has to be an integer).

We now need to account for the possibility that $D_B(\alpha)$ has an eigenvalue on ∂F . Periodicity of the spectrum shows that if $k_1 \in \text{Spec } D_B(\alpha) \cap \partial F$ then $k_1 + \gamma \in \partial F$ for a finite number of $\gamma \in \Lambda^*$ (from the definition of a fundamental domain). Only one of these points can be in the fundamental domain F and a small deformation includes it in the interior of (the new) F , while excludes all others from ∂F . The previous argument shows that the number of eigenvalues remains 2. \square

Proof of Theorem 3. When $B, \alpha \in \mathbb{R}$ then the last identity in (2.10) gives

$$\text{Spec}_{L_0^2} D_B(\alpha) = -\text{Spec}_{L_0^2} D_B(\alpha) = \overline{\text{Spec}_{L_0^2} D_B(\alpha)}. \quad (6.4)$$

From Theorem 1 we know that for $\alpha \notin \mathcal{A}$,

$$\text{Spec}_{L_0^2}(D_B(\alpha)) = \{d(\alpha), -d(\alpha)\} + \Lambda^*$$

(we fix $B \in \mathbb{R}$ here) and (6.4) shows that

$$\overline{d(\alpha)} \equiv d(\alpha) \pmod{\Lambda^*} \quad \text{or} \quad \overline{d(\alpha)} \equiv -d(\alpha) \pmod{\Lambda^*}.$$

Since $\overline{\Lambda^*} = \Lambda^*$ this means that $\text{Spec}_{L_0^2} D_B(\alpha) \subset (\mathbb{R} + \Lambda^*) \cup (i\mathbb{R} + \Lambda^*)$ which is the same as (2.17).

To prove (2.18) we recall that $\mathbb{C} \times (\mathbb{C} \setminus \mathcal{K}_0) \ni (B, k) \mapsto T_k(B)$, is a holomorphic family of compact operators with simple eigenvalue $\mu = 1/\underline{\alpha} \in \text{Spec}(T_k(0))$. We define $\mathcal{H} := \mathcal{R} \setminus \bigcup_{k' \in \mathcal{K}_0} D(k', \varepsilon)$, then by periodicity of the spectrum of $D_B(\alpha)$ it suffices to

restrict us to a fundamental domain: Since \mathcal{K}/Λ^* is a compact set, the spectrum of $\mathcal{K} \ni k \mapsto T_k(B)$ is uniformly continuous in B on compact sets. Thus, for $0 < |B| < \delta_0$ small enough, the operator $T_k(B)$ has precisely one eigenvalue in a δ_1 neighbourhood of μ for every k . This implies that for every $k \in \mathcal{K}/\Lambda^*$ there is precisely one μ_k such that $\mu_k \in \text{Spec}(T_k(B))$ and $|\mu_k - \mu| < \delta_1$. From Propositions 5.1 and 5.3 we conclude that $\mu_k \in \mathbb{R}$ and the result follows. \square

Remark. While our proof does not show that for $B \in \mathbb{R} \setminus \{0\}$ the points K, K' are also in the spectrum of $D_B(\alpha)$ for some real α between successive magic angle, the bottom figure in Figure 8 shows that this is indeed the case. For general $B \notin \mathbb{R}$ this is however false, as the top figure in Figure 8 shows. Both figures exhibit an interesting universal pattern for $|\alpha|$ large.

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Email address: `simon.becker@math.ethz.ch`

ETH ZURICH, INSTITUTE FOR MATHEMATICAL RESEARCH, RÄMISTRASSE 101, 8092 ZURICH, SWITZERLAND

Email address: `zworski@math.berkeley.edu`

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF CALIFORNIA, BERKELEY, CA 94720, USA