J. Spectr. Theory 14 (2024), 479–511
DOI 10.4171/JST/504

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 realised [8] theoretical prediction [6] of a *magic* angle of twisting at which TBG acquires special properties. These special properties are due to the existence of nearly flat bands of the corresponding periodic spectral problem. Tarnopolsky–Kruchkov–Vishwanath [18] 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 [20] and Becker et al. [1–3].

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

Mathematics Subject Classification 2020: 35J10 (primary); 81Q05, 81Q12, 81Q70 (secondary).
Keywords: condensed matter physics, Dirac operators, spectral theory, magnetic fields, moiré materials, twisted bilayer graphene.

papers by Kwan et al. [13] and Qin–MacDonald [15] (see also [16]) 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 find that the two 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 Section 3.7 for the discussion of simplicity.) For the Bistritzer–MacDonald potential $U_{\mathrm{BM}}(z)$ (see the caption of 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 [18]. That is, it 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 (see Figure 4): 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[1] 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 Section 3.1) – for the discussion of such phenomena in the physics literature, see [9, 13, 14].
- 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

[1] https://math.berkeley.edu/∼zworski/magic_billiard.mp4, visited on 10 June 2024.

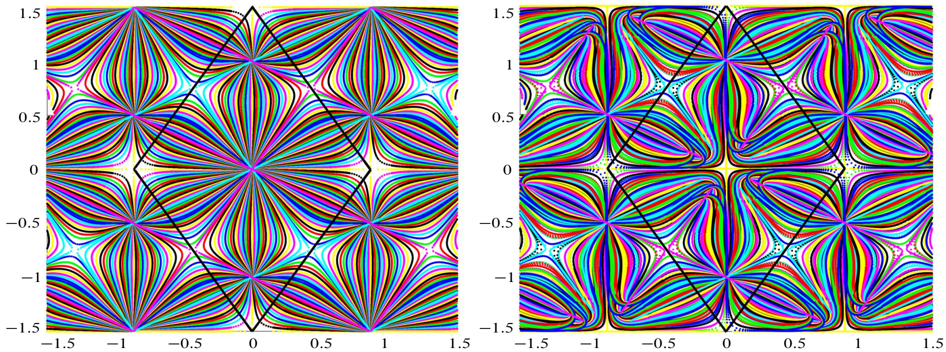

Figure 1. We show the movement of Dirac points as α varies in $(0, 2.3)$ for the Bistritzer–MacDonald potential $U(z) = U_{\mathrm{BM}} = \sum_{k=0}^{2} \omega^k e^{\frac{1}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}$ (left) and $\alpha \in (0, 2.7)$ and $U(z) = 2^{-\frac{1}{2}}(U_{\mathrm{BM}}(z) - \sum_{k=0}^{2} \omega^k e^{-z\bar{\omega}^k - \bar{z}\omega^k})$ (right). (Here, we use the convention of [1,18] – see (2.4).) 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[2] and[3] for the corresponding animations.

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 organised as follows.

- We present the Hamiltonian and the definition of Dirac points in Section 2. We also establish basic symmetry properties of Dirac points and a perturbation result valid away from magic α's.
- In Section 3, we review the theory of magic angles following [1,3] but in a more invariant and general way.
- In Section 4, we set up Grushin problems needed for understanding the small in-plane magnetic fields as a perturbation.
- We then specialise, in Section 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 Section 6 with the proofs of the main theorems.

[2] https://math.berkeley.edu/∼zworski/B01.mp4, visited on 10 June 2024.
[3] https://math.berkeley.edu/∼zworski/B01_double.mp4, visited on 10 June 2024.

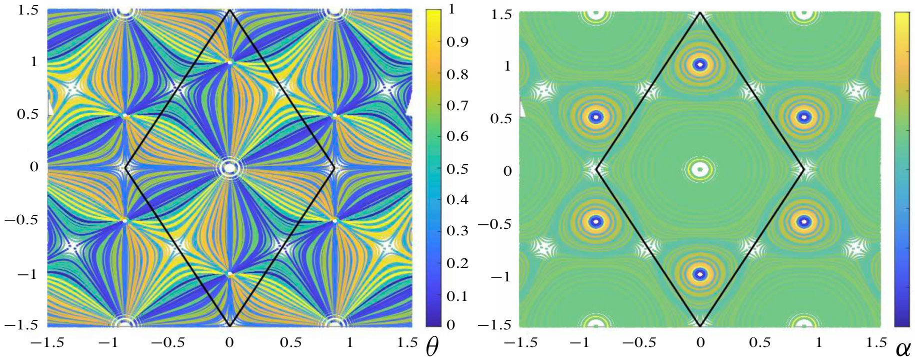

Figure 2. The dynamics of Dirac points for the Bistritzer–MacDonald potential $U(z) = U_{\mathrm{BM}} = \sum_{k=0}^{2} \omega^k e^{\frac{1}{2}(z\bar\omega^k - \bar z \omega^k)}$. The magnetic field given by $B = B_0 e^{2\pi i\theta}$ with $B_0 = 0.1$ On the left, different colours correspond to different 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[4] for $E_1(\alpha, k)/\max_k E_1(\alpha, k)$ for fixed B as α varies.

2. In-plane magnetic field

Adding a constant in-plane magnetic field [13, 15] 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 [18] results for layers at positions $z_\perp = \pm 1$, in the Hamiltonian $H_B(\alpha)$ in (2.5), built from non-normal operators

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

where we make the following assumptions on U:

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

[4] https://math.berkeley.edu/∼zworski/first_band.mp4, visited on 10 June 2024.

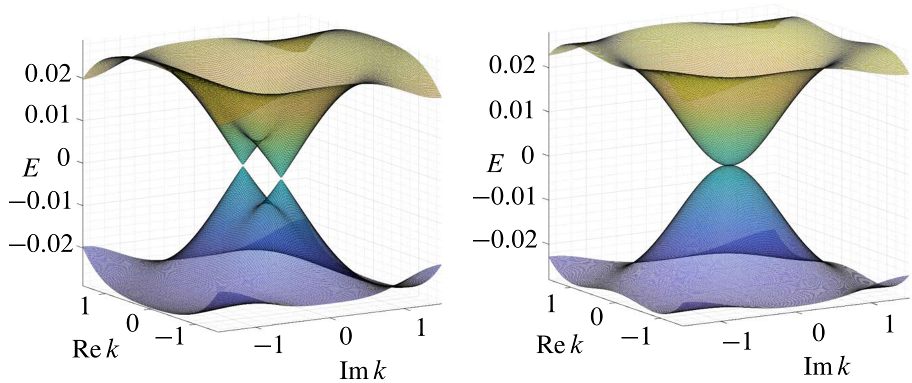

Figure 3. When B is real (in the convention of (2.1)), two Dirac cones approach Γ point as $\alpha \to \alpha^* = \underline{\alpha} + \mathcal{O}(B^3)$ ($\underline{\alpha}$ a simple real magic parameter) on the line $\operatorname{Im} k = 0$ (left). For $\alpha = \alpha^*$, the quasi-momentum k at which the bifurcation happens are the boundary of the Brillouin zone and the Γ-point which is shown in the figure (right). The animation[5] shows the motion of Dirac points in this case.

In this convention, the Bistritzer–MacDonald potential used in [1, 18] corresponds to

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

For a discussion of a perpendicular constant magnetic field in the chiral model of twisted bilayer graphene, we refer to [5].

Remark. We adapt here a more mathematically straightforward convention of coordinates than that of [1, 2], where we followed [18] (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 [1] and rigorously derived in [7, 19] was

$$\begin{gathered}\widetilde{D}(\alpha) := \begin{pmatrix} 2D_{\bar\zeta} & \alpha U_0(\zeta) \\ \alpha U_0(-\zeta) & 2D_{\bar\zeta}\end{pmatrix}, \quad \overline{U_0(\bar\zeta)} = U_0(\zeta), \\ U_0\Big(\zeta + \frac{4\pi i}{3}(a_1\omega + a_2\omega^2)\Big) = \bar\omega^{a_1+a_2} U_0(\zeta), \quad U_0(\omega\zeta) = \omega U_0(\zeta).\end{gathered} \tag{2.3}$$

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

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

[5] https://math.berkeley.edu/∼zworski/Rectangle_1.mp4, visited on 10 June 2024.

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

$$\zeta = \frac{4}{3}\pi i z, \quad \frac{1}{3}\Gamma = \frac{4}{3}\pi i \Lambda, \quad 3\Gamma^* = \left(\frac{1}{3}\Gamma\right)^* = \sqrt{3}\Lambda = \frac{3}{4\pi i}\Lambda^*. \tag{2.4}$$

Then,

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

The twisted periodicity condition in (2.3) corresponds to the condition in (2.2) since $\bar\omega^{a_1+a_2} = e^{i\langle a_1\omega + a_2\omega^2, K\rangle}$, $K = 4\pi i(-\frac{1}{3} - \frac{2}{3}\omega)/\sqrt{3} = 4\pi/3$. See the caption of Figure 1 for examples of $U_0(z)$ in the coordinates of [1, 18].

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

$$H_B(\alpha) = \begin{pmatrix} 0 & D_B(\alpha)^* \\ D_B(\alpha) & 0 \end{pmatrix}, \tag{2.5}$$

and the Dirac points are given by the spectrum of

$$D_B(\alpha) : H_0^1 \to L_0^2,$$
$$L_0^2 := \left\{u \in L^2_{\rm loc}(\mathbb{C};\mathbb{C}) : u(x+\gamma) = \operatorname{diag}\left(e^{-i\langle\gamma,K\rangle}, e^{i\langle\gamma,K\rangle}\right)u(x)\right\},$$

with a similar definition of H_0^1 (replace $L^2_{\rm loc}$ with $H^1_{\rm loc}$) – see Section 3.1 for a systematic discussion and explanations.

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

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

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 $\alpha^{-1} \in \operatorname{Spec}_{L_0^2} T_k$, where $\mathbb{C} \setminus \{K, -K\} \mapsto T_k$ is a (holomorphic) family of compact operators given in (3.18). (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 Section 3.7):

$$\alpha \in \mathcal{A} \text{ is said to be simple} \Leftrightarrow 1/\alpha \text{ is a simple eigenvalue of } T_k. \tag{2.6}$$

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

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

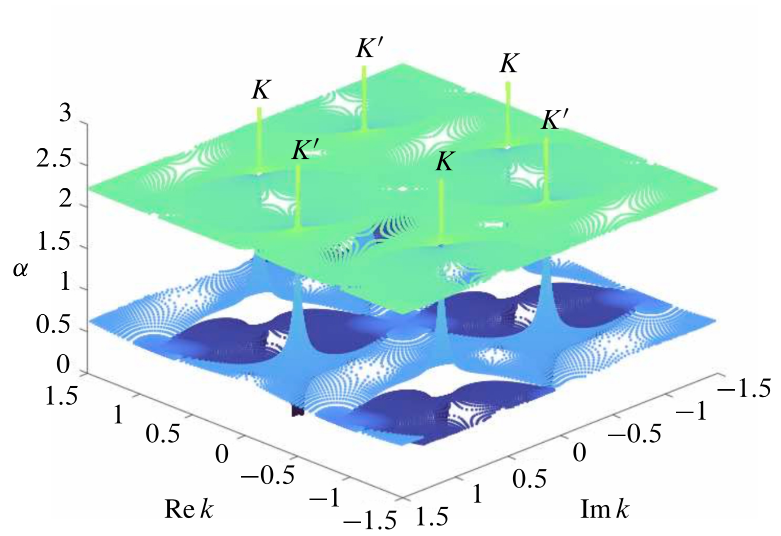

Figure 4. Dirac point dynamics for $B = 0.1e^{2\pi i\theta}$ with $\theta \in [0, 1/2]$. Close to the first two magic angles ($\alpha \approx 0.585, 2.221$), the dynamics spreads out in space.

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*

$$\operatorname{Spec}_{L^2_0}(D_B(\alpha)) = (k_B(\alpha) + \Lambda^*) \cup (-k_B(\alpha) + \Lambda^*),$$

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

$$\begin{aligned} \operatorname{Spec}_{L^2_0} D_{\omega B}(\alpha) &= \omega \operatorname{Spec}_{L^2_0} D_B(\alpha), \\ \operatorname{Spec}_{L^2_0} D_B(-\alpha) &= \operatorname{Spec}_{L^2_0} D_B(\alpha) = -\operatorname{Spec}_{L^2_0} D_B(\alpha), \\ \operatorname{Spec}_{L^2_0} D_{\bar{B}}(\bar{\alpha}) &= \overline{\operatorname{Spec}_{L^2_0} D_B(\alpha)}. \end{aligned} \tag{2.7}$$

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

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

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

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

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 (2.7). We now recall the following antilinear symmetries:

$$FD(\alpha)F = D(-\bar{\alpha}), \quad Fv(z) := \overline{v(-\bar{z})},$$

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

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 $k \mapsto -k$)

$$\operatorname{Spec}_{L^2_0}(D_B(\alpha)) = \overline{\operatorname{Spec}_{L^2_0}(D_{\bar{B}}(-\bar{\alpha}))} = \operatorname{Spec}_{L^2_0}(D_B(-\alpha)),$$

and that gives the rest of (2.7). ∎

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

Theorem 2. *Suppose that $\underline{\alpha} \in \mathcal{A}$ 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^2_0 is discrete and*

$$|\operatorname{Spec}_{L^2_0}(D_B(\alpha)) \cap \mathbb{C}/\Lambda^*| = 2, \tag{2.8}$$

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 $0 < |B| < \delta$, $|\alpha - \underline{\alpha}| < a_0\delta|B|$,

$$\operatorname{Spec}_{L^2_0}(D_B(\alpha)) \subset \Lambda^* + D(0, \varepsilon), \tag{2.9}$$

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 [20] and its simplicity (including the simplicity as an eigenvalue of the operator T_k defined in (3.18)) in [2], 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 [18].

(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

Magic angle $\underline{\alpha}$	0.585	2.221	3.751	5.276	6.794	8.312	9.829
$\lvert g_0(\underline{\alpha})\rvert \simeq$	7e-02	5e-04	7e-04	2e-05	3e-05	9e-07	6e-06
$\lvert g_1(\underline{\alpha})\rvert \simeq$	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.

are the results for the (numerically) simple magic angles for the potential U_{BM} in Table 1.

(3) The combination of Theorems 1 and 2 shows that for any $U \Subset (\mathbb{C} \setminus \mathcal{A}) \cup \{\underline{\alpha}\}$ (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

$$|\mathrm{Spec}_{L_0^2}(D_B(\alpha)) \cap \mathbb{C}/\Lambda^*| = 2.$$

From the symmetries in (2.7), 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 (2.7) to obtain the other two.

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

$$\mathrm{Spec}_{L_0^2}(D_B(\alpha)) \subset \mathcal{R} := 2\pi(i\mathbb{R} + \mathbb{Z}) \cup \frac{2\pi}{\sqrt{3}}(\mathbb{R} + i\mathbb{Z}), \quad \alpha \in \mathbb{R} \setminus \mathcal{A}. \tag{2.10}$$

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*

$$\mathcal{R} \setminus \bigcup_{k \in \mathcal{K}_0} D(k, \varepsilon) \subset \bigcup_{\underline{\alpha}-\delta_1<\alpha<\underline{\alpha}+\delta_1} \mathrm{Spec}_{L_0^2}(D_B(\alpha)) \subset \mathcal{R}, \quad 0 < B < \delta_0. \tag{2.11}$$

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* $k \in \mathrm{Spec}_{L_0^2}(D_B(\alpha))$.

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 (5.12).

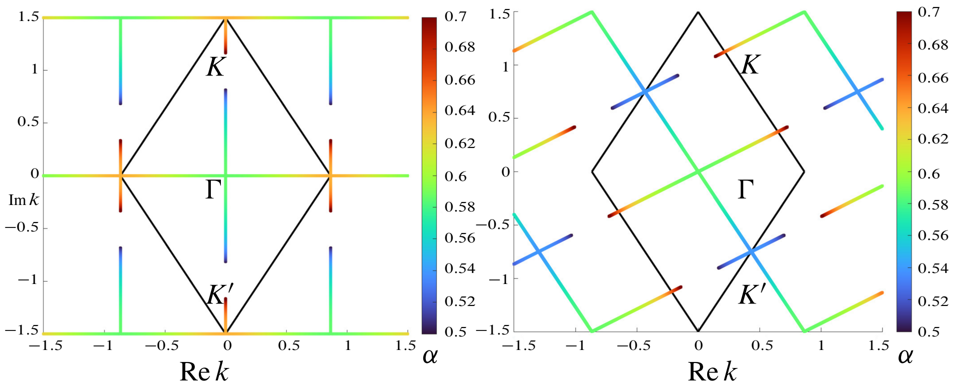

Figure 5. Dirac point trajectory for $B = 0.1$ (left) and $B = 0.1\omega$ (right). The bifurcation happens at Γ and one additional point (modulo Λ^*) in each figure, respectively. The colours indicate the position of the Dirac cones for given values of α. The exclusion of K and K' points in the statement of Theorem 3 seems to be a technical issue, as shown in[6] (for the case of the figure on the right).

(2) The inclusion (2.10) means that the spectrum lies on a grid of straight lines parallel to the x- and y-axes – see[7] and Figure 5. To obtain the sets of other rectangles, we use the first identity in (2.7); that is, take $B = \omega B_0$, $B_0 > 0$.

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 generalisation of (2.1):

$$D(\alpha) := 2D_{\bar{z}} + \alpha V(z) : H^1_{\mathrm{loc}}(\mathbb{C}; \mathbb{C}^n) \to L^2_{\mathrm{loc}}(\mathbb{C}; \mathbb{C}^n), \quad H(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* \\ D(\alpha) & 0 \end{pmatrix},$$

[6]https://math.berkeley.edu/~zworski/Rectangle_2.mp4, visited on 10 June 2024.
[7]https://math.berkeley.edu/~zworski/Rectangle_1.mp4, visited on 10 June 2024.

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

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

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

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

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

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

If we define

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

then

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

and

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

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

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

We have

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

Thus, we can define a generalised Bloch transform

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

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

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

We check that

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

and that

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

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

$$H_0^s = H_0^s(\mathbb{C};\mathbb{C}^k) := \{u \in H^s_{\mathrm{loc}}(\mathbb{C};\mathbb{C}^k) : \mathscr{L}_\gamma u = u,\ \gamma \in \Lambda\}, \quad L_0^2 := H_0^0,\ k = n, 2n.$$

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

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

where we used the notation of (3.4).

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

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

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

$$\tau(p) : L_0^2 \to L_0^2, \quad [\tau(p)u](z) := e^{i\langle z,p\rangle}u(z), \quad \tau(p)^{-1} = \tau(p)^* \tag{3.6}$$

and

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

we have

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

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

$$\mathrm{Spec}_{L_0^2}(2D_{\bar z}) = \bigsqcup_{j=1}^{n}(\Lambda^* - k_j), \quad \text{Domain of } 2D_{\bar z} = H_0^1. \tag{3.7}$$

3.2. Rotational symmetries

We now introduce

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

and in addition to (3.1) assume that

$$V(\omega z) = \omega V(z). \tag{3.8}$$

(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

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

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

$$\rho(\gamma) = \rho(\omega\gamma), \quad \forall \gamma \in \Lambda, \tag{3.9}$$

which implies that

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

In the notation of (3.2), condition (3.9) means that

$$\bar\omega k_j \equiv k_j \bmod \Lambda^* \Leftrightarrow k_j \in \mathcal{K} := \frac{4\pi i}{\sqrt{3}}\left(\left\{0, \pm\left(\frac{1}{3} + \frac{2}{3}\omega\right)\right\} + \Lambda\right).$$

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

Since (3.9) 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 [1, Section 2.1] and combine the two actions into a group of unitary action which commute with $H(\alpha)$:

$$\begin{aligned} G &:= \Lambda \rtimes \mathbb{Z}_3, \quad \mathbb{Z}_3 \ni \ell : \gamma \to \bar\omega^\ell\gamma, \\ (\gamma,\ell)\cdot(\gamma',\ell') &= (\gamma + \bar\omega^\ell\gamma', \ell + \ell'), \\ (\gamma,\ell)\cdot u &= \mathcal{L}_\gamma\mathcal{C}^\ell u, \quad u \in L^2_{\mathrm{loc}}(\mathbb{C};\mathbb{C}^n \times \mathbb{C}^n). \end{aligned} \tag{3.10}$$

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 $H(\alpha)$:

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

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

$$\begin{aligned} &H(\alpha) = -\mathcal{W} H(\alpha) \mathcal{W}, \quad \mathcal{W} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} : \mathbb{C}^n \times \mathbb{C}^n \to \mathbb{C}^n \times \mathbb{C}^n, \\ &\mathcal{W}\mathcal{C} = \mathcal{C}\mathcal{W}, \quad \mathcal{L}_\gamma \mathcal{W} = \mathcal{W} \mathcal{L}_\gamma. \end{aligned} \tag{3.11}$$

3.3. Protected states

We now make the assumption (3.9) and consider the question of protected states. We are looking for the set $\mathcal{K}_0 \subset \mathbb{C}$ such that

$$\forall \alpha \in \mathbb{C}, \quad k \in \mathcal{K}_0, \quad 0 \in \operatorname{Spec}_{L^2_0} H_k(\alpha). \tag{3.12}$$

This condition is equivalent to

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

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:

$$H^s_k := \{u \in H^s(\mathbb{C}/3\Lambda; \mathbb{C}^2 \times \mathbb{C}^2) : \mathcal{L}_\gamma u = e^{i\langle k,\gamma\rangle} u\}, \quad k \in \mathcal{K}/\Lambda^* \simeq \mathbb{Z}^3, \ p \in \mathbb{Z}^3, \tag{3.13}$$

(with the corresponding definition of L^2_k).

Lemma 3.1. *Suppose that $k, k' \in \mathcal{K}$ and $\tau(k)$ is defined as in (3.6). Then, in the notation of (3.13), $\tau(k) : H^s_{k'} \to H^s_{k'+k}$ and*

$$\begin{aligned} \tau(k) &: \ker_{H^1_0}(D(\alpha) + k) \to \ker_{H^1_k} D(\alpha), \\ \tau(k) &: \ker_{H^1_0} H_{-k}(\alpha) \to \ker_{H^1_k} H(\alpha). \end{aligned} \tag{3.14}$$

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

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

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, $w \in H^1_k$. ∎

We are interested in the case of $n = 2$ and obtain the following reinterpretation of earlier statements about protected states – see [18].

Proposition 3.2. *If $n = 2$ (in the notation of (3.2) and (3.12)) and $k_1 \not\equiv k_2 \bmod \Lambda^*$, $k_j \in \mathcal{K}$, then $\mathcal{K}_0 = \{-k_1, -k_2\} + \Lambda^*$.*

Proof. We use (3.14) and decompose $\ker_{H^1(\mathbb{C}/3\Lambda;\mathbb{C}^4)} H(\alpha)$ into representations of G_3 given by (3.10). From (3.11), we see that the spectrum of $H(\alpha)$ restricted to a representation of G_3 is symmetric with respect to the origin. If (see [1, Section 2.2] for a review of representations of G_3)

$$H^s_{k,p} := \{u \in H^s(\mathbb{C}/3\Lambda; \mathbb{C}^2 \times \mathbb{C}^2) : \mathcal{L}_\gamma \mathcal{C}^\ell u = e^{i\langle k,\gamma\rangle} \bar{\omega}^{\ell p} u\}, \tag{3.15}$$

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

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

and since $k_1 \not\equiv k_2 \bmod \Lambda^*$, all these spaces are different. The spectrum of $H(\alpha)|_{L^2_{k,p}}$ is even (see (3.11)) and $\ker_{H^1_{k_j,p}} H(0) = \mathbb{C}\mathbf{e}_{j+2p}$, $j = 1, 2$, $p = 0, 1$. Continuity of eigenvalues shows that

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

which in view of Lemma 3.1 concludes the proof. ∎

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 $\mathcal{K}/\Lambda^*$ is called the Γ point.

Existence of protected states shows that we have a natural labelling for the eigenvalues of $H(k)$ on L^2_0:

$$\begin{aligned} &\operatorname{Spec}_{L^2_0}(H(k)) = \{E_j(\alpha, k)\}_{j \in \mathbb{Z}^*}, \quad E_j(\alpha, k) = -E_{-j}(\alpha, k), \\ &0 \leq E_1(\alpha, k) \leq E_2(\alpha, k) \leq \cdots, \quad E_{\pm 1}(\alpha, -k_1) = E_{\pm 1}(\alpha, -k_2) = 0, \end{aligned} \tag{3.16}$$

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 [1], the spectral characterisation of *magic angles*. See also proof of [3, Proposition 2.2].

Proposition 3.3. *Suppose that $n = 2$ and that the condition (3.9) holds. Then, in the notation of Proposition 3.2, there exists a discrete set $\mathcal{A}$ such that*

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

Moreover,

$$\alpha \in \mathcal{A} \Leftrightarrow \exists k \notin \mathcal{K}_0, \quad \alpha^{-1} \in \operatorname{Spec}_{L^2_0} T_k \Leftrightarrow \forall k \notin \mathcal{K}_0, \quad \alpha^{-1} \in \operatorname{Spec}_{L^2_0} T_k, \tag{3.17}$$

where T_k is a compact operator given by

$$T_k := R(k)V(z) : L^2_0 \to L^2_0, \quad R(k) := (2D_{\bar z} - k)^{-1}. \tag{3.18}$$

3.5. Antilinear symmetry

We will make the following assumption:

$$\mathcal{A}D(\alpha) = -D(\alpha)^*\mathcal{A}, \quad \mathcal{A} := \begin{pmatrix} 0 & \Gamma \\ -\Gamma & 0 \end{pmatrix}, \quad \Gamma v(z) = \overline{v(z)}. \tag{3.19}$$

A calculation based on the definition of $\mathcal{L}_\gamma$ gives

$$\mathcal{A} : L^2_{k,p} \to L^2_{-k+k_1+k_2,-p}, \quad k \in \mathcal{K}, \ p \in \mathbb{Z}_3. \tag{3.20}$$

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

$$-k_0 + k_1 + k_2 \equiv k_0 \bmod \Lambda^*,$$

and consequently,

$$\mathcal{A} : L^2_{k_0,p} \to L^2_{k_0,-p}, \quad p \in \mathbb{Z}_3. \tag{3.21}$$

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 (3.19) 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 (3.8), we see that $W_1(\omega z) = \omega W_1(z)$ and hence the integral of W_1 over $\mathbb{C}/\Lambda$ 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 (3.19), then we can, without loss of generality, assume that

$$\begin{aligned} V(z) &= \begin{pmatrix} 0 & V_{12}(z) \\ V_{21}(z) & 0 \end{pmatrix}, \\ V_{ij}(z+\gamma) &= e^{i\langle k_j - k_i, \gamma\rangle} V_{ij}(z), \quad k_\ell \in \mathcal{K},\ k_1 \neq k_2, \\ V_{ij}(\omega z) &= \omega V_{ij}(z). \end{aligned} \tag{3.22}$$

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:

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

The mapping property is simpler than (3.20):

$$Q : L^2_{k,p}(\mathbb{C}/\Lambda; \mathbb{C}^2) \to L^2_{k,-p}(\mathbb{C}/\Lambda; \mathbb{C}^2).$$

3.6. Theta functions

We now review some properties of theta functions. To simplify notation, we put

$$\theta(z) := \theta_1(z|\omega) := -\theta_{\frac12,\frac12}(z|\omega),$$

and recall that

$$\begin{aligned} &\theta(z) = -\sum_{n\in\mathbb{Z}} \exp\left(\pi i \left(n+\frac12\right)^2 \omega + 2\pi i \left(n+\frac12\right)\left(z+\frac12\right)\right), \quad \theta(-z) = -\theta(z) \\ &\theta(z+m) = (-1)^m \theta(z), \quad \theta(z+n\omega) = (-1)^n e^{-\pi i n^2\omega - 2\pi i z n}\theta(z), \end{aligned} \tag{3.23}$$

and that θ has simple zeros at Λ (and no other zeros) – see [12].

We now define

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

Then, using (3.23) and differentiating in the sense of distributions,

$$\begin{aligned} F_k(z+m+n\omega) &= e^{-nk\,\mathrm{Im}\,\omega} e^{2\pi i n z(k)} F_k(z) = F_k(z), \\ (2D_{\bar z}+k)F_k(z) &= c(k)\delta_\Lambda(z), \quad c(k) := 2\pi i\theta(z(k))/\theta'(0). \end{aligned} \tag{3.24}$$

(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, [11, (3.1.12)].)

The following Lemma is now immediate. It reinterprets the theta function argument in [18].

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

$$(D(\alpha)+k+k')(F_{k'}(z-z(k''))u(z)) = c(k'-k'')\delta_{z(k'')}(z)u(z(k'')), \quad k,k',k''\in\mathbb{C}, \tag{3.25}$$

where $c(k)$ *is given in* (3.24). *In particular, if* $u(z(k''))=0$, *then*

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

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[8]. One natural definition of multiplicity of magic angles is given in terms of eigenvalues of $H_k(\alpha)$ in (3.16). We first note that

$$\alpha\in\mathcal{A} \Leftrightarrow \forall k\in\mathbb{C}/\Lambda^*, \quad E_{\pm1}(\alpha,k)=0. \tag{3.26}$$

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

$$\forall k\in\mathbb{C},\ j>1, \quad E_j(\alpha,k)>0. \tag{3.27}$$

As stated in (2.6), we use a stronger definition in this paper.

The operators

$$\mathbb{C}^2 \ni (\alpha,k)\mapsto D(\alpha)+k : H^1_0\to L^2_0$$

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 (3.26) implies that $D(\alpha)-k$ is invertible for some k and α.) In particular,

$$\dim\ker(D(\alpha)+k) = \dim\operatorname{coker}(D(\alpha)^*+\bar k) = \dim\ker(D(\alpha)^*-\bar k),$$

[8] A more general discussion is presented in [4] – generic simplicity presented there is modified in view of protected multiplicity two magic angles – see the proof of Proposition 3.6.

and hence,

$$(3.27) \Leftrightarrow \forall k \in \mathbb{C}, \quad \dim \ker_{H_0^1}(D(\alpha) + k) = 1.$$

In [3, Theorem 2], we proved that

Proposition 3.5. *Suppose that* (3.22) *holds and that*

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

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

$$(3.27) \Leftrightarrow \exists k \not\equiv k_1, k_2 \bmod \Lambda^*, \quad \dim \ker_{H_0^1}(D(\alpha) + k) = 1.$$

In particular, $\alpha \in \mathbb{C}$ *is a simple magic angle (in the sense of* (3.27)*) if and only if*

$$\dim \ker_{H_0^1}(D(\alpha) + k_0) = 1. \tag{3.28}$$

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

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

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

This corresponds to $\Gamma = 0$ in the physics notation. In [1], we followed [18] and used a non-symmetric (equivalent) choice. This corresponds to the assumptions in (2.2) with

$$k_1 = K.$$

Proposition 3.6. *Suppose that* (3.28) *holds. Then, in the notation of Lemma* 3.1,

$$\ker_{H_0^1}(D(\alpha) + k_0) = \mathbb{C}\tau(k_0)^* u_0, \quad \|u_0\|_{L^2_{k_0}} = 1, \ \Omega u_0 = \omega u_0; \tag{3.29}$$

that is, in the notation of (3.15), $u_0 \in L^2_{k_0,2}$. *In addition,*

$$u_0(z) = z w(z), \quad w \in C^\infty(\mathbb{C}; \mathbb{C}^2), \quad w(0) \neq 0, \quad u_0(z) \neq 0, \quad z \notin \Lambda. \tag{3.30}$$

Remark. The key insight in [18] was to use vanishing of $u \in \ker_{H^1_{k_1}} D(\alpha)$ for magic α's at a distinguished point z_S to show that $\mathrm{Spec}_{H_0^1}(D(\alpha)) = \mathbb{C}$. In [1, Theorems 1], this was shown to be equivalent to the spectral definition based on Proposition 3.3. Here, we take a direct approach: only at magic α's we have $\ker_{H^1_{k_0}} D(\alpha) \neq \{0\}$ and (3.29) shows that its elements have to vanish at 0. Equation (3.25) then implies vanishing of other eigenfunctions.

Proof of Proposition 3.6. From Lemma 3.1 and (3.28), we conclude that

$$\ker_{H^1_{k_0}} D(\alpha) = \mathbb{C} u_0$$

and as $L^2_{k_0} = \bigoplus_{j=0}^2 L^2_{k_0,j}$ we can decompose the kernel using these subspaces. Since $D(0) + k_0 : H^1_0 \to L^2_0$ is invertible (see (3.7)), (3.14) shows that

$$D(0) : H^1_{k_0} \to L^2_{k_0}$$

is invertible with the inverse given by $R(0)$. It then follows that (see (3.18))

$$I + \alpha T_0 = R(0)D(\alpha) : L^2_{k_0,j} \to L^2_{k_0,j}, \quad \ker_{H^1_{k_0,j}} D(\alpha) = \ker_{L^2_{k_0,j}} R(0)D(\alpha).$$

(We do use ellipticity of $D(\alpha)$ here: the element of the kernel on L^2 must automatically be smooth.) Hence, if $\ker_{L^2_{k_0,j}}(R(0)D(\alpha)) \neq \{0\}$, $j = 0, 1$, then

$$\ker_{L^2_{k_0,j}}(D(\alpha)^* R(0)^*) \neq \{0\},$$

and there exists $w \in L^2_{k_0,j}$ such that $D(\alpha)^* R(0)^* w = 0$. We now note that

$$R(0)^* : L^2_{k_0,j} \to L^2_{k_0,j-1}. \tag{3.31}$$

In fact, $2D_{\bar{z}} = D(0) : H^1_{k_0} \to L^2_{k_0}$ is invertible by Propositions 3.2 and 3.3 and

$$R(0) : L^2_{k_0} \to H^1_{k_0} \subset L^2_{k_0}$$

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 (3.15), $2D_{\bar{z}} : H^1_{k_0,j} \to L^2_{k_0,j-1}$. Consequently, $R(0) : L^2_{k_0,j-1} \to L^2_{k_0,j}$ and as the dual space to $L^2_{k_0,p}$ (using the L^2 pairing) is given by $L^2_{k_0,p}$, (3.31) follows.

This and $\mathscr{A} : L^2_{k_0,j-1} \to L^2_{k_0,-j+1}$ (see (3.21)) show that

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

This means that $\dim \ker_{H^1_{k_0}} D(\alpha) > 1$, contradicting the simplicity assumption. The simplicity and uniqueness of the zero of u_0 (3.30) follow from [3, Theorem 3]. ∎

For an $\alpha \in \mathcal{A}$, we assume that (3.28) holds. In that case, Proposition 3.6 and Lemma 3.4 show that

$$\ker_{H^1_0}(D(\alpha) + k) = \mathbb{C} u(k), \quad u(k) := \frac{F_k u_0}{\|F_k u_0\|}. \tag{3.32}$$

Using (3.19), we see that (since $\mathcal{A}^2 = -I$)

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

which implies that

$$\ker_{H_0^1}(D(\alpha)^* + \bar{k}) = \mathbb{C}\mathcal{A}u(-k). \tag{3.33}$$

Remark. From [3, (6.6)], we see that (note the difference of notation: $u(k)$ there is not normalised), for the basis of Λ^* satisfying $z(e_1) = 1$, $z(e_2) = \omega$, we have, for $p = me_1 + ne_2 \in \Lambda^*$,

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

where the unitary operator $\tau(p)$ was defined in (3.6).

4. Grushin problems

In this section, we construct Grushin problems (see [17] and [10, Section C.1]) which allow us to treat small in-plane magnetic fields as perturbations. In Section 5, we combine that with the spectral characterisation of magic angles (Proposition 3.3) to analyse 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 that $\underline{\alpha} \in \mathcal{A}$ is simple, in the sense that (3.28) holds. We then put, in the notation of (3.32) and (3.33),

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

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

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

We now apply [10, Lemma C.3] to obtain

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

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-normalisations 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 [12, (4.7a)])

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

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

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

this integral vanishes, and (4.4) gives

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

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 [17, Proposition 2.12])

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

where and in the notation following (4.3),

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

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):

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

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 $\widetilde{E}_\bullet^B(k,\alpha,z)$, and we have

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

Using [10, Lemma C.3] again, we see that (in the notation of (4.6))

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

(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 normalisation 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 to 0) for k close to 0 are given by solutions of

$$\det \widetilde{E}_\pm^B(k,\alpha,z) = 0 \Rightarrow$$
$$z = \pm\left|\gamma_1 Bk^2 + \gamma_0(\alpha - \underline{\alpha}) + \mathcal{O}(|B|^2 + |\alpha - \underline{\alpha}|^2 + |k|^4)\right|, \tag{4.9}$$

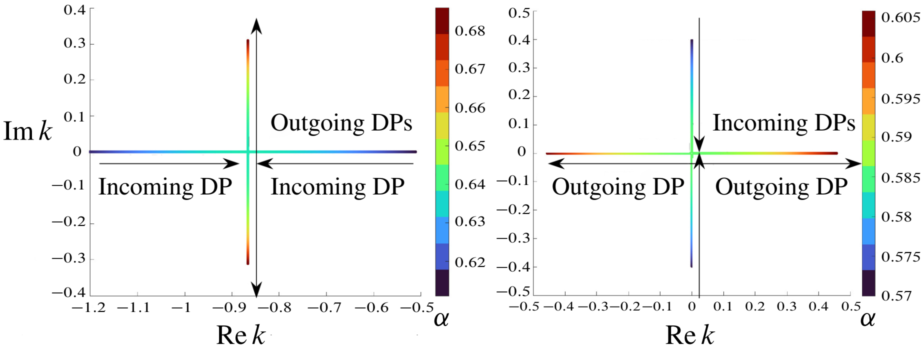

Figure 6. Bifurcation for $B = 0.1$. (Top): the colour-coding indicates the position of the Dirac points for given values of $\alpha \in \mathbb{R}$. The right figure illustrates the bifurcation at Γ and the left figure at a non-equivalent (modulo Λ^*) bifurcation point that is a vertex of the boundary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

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 (3.11) to the Grushin problem (4.8) which shows that $\det \widetilde{E}_{\pm}^{B}(k, \alpha, z) = \det \widetilde{E}_{\pm}^{B}(k, \alpha, -z)$.)

5. Bifurcation

This section is devoted to showing (2.11) and giving a stronger version of Theorem 3.

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

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

and we can define

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

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

$$k \in \operatorname{Spec}_{L_0^2}(D_B(\alpha)) \Leftrightarrow 1/\alpha \in \operatorname{Spec}_{L_0^2}(T_k(B)). \tag{5.2}$$

In particular, this characterisation 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 characterisation with the result of Section 4, we can obtain a rather precise characterisation 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 exist $\delta > 0$ and a holomorphic function $\lambda(k, B)$ such that $\lambda(k, B)$ is a simple eigenvalue of $T_k(B)$ and*

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

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

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

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

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 $0 < |B| \ll 1$, $k \in \operatorname{Spec}_{L_0^2} D_B(\alpha) \cap D(0, \delta)$, $0 < \delta \ll 1$, if and only if

$$
B k^2 (1 + \mathcal{O}(k^6) + \mathcal{O}(B^3) + \mathcal{O}(B k^2)) = c_1^{-1} (1 - \alpha/\underline{\alpha} + B^3 \lambda_1(B^3)). \tag{5.5}
$$

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 (2.7).

(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 $k \in U$, $T_k(B) = T_k(0) + \mathcal{O}(B)_{L_0^2 \to L_0^2}$, and if $0 < \varepsilon_0 \ll 1$, then the projection,

$$
\Pi(k, B) := (2\pi i)^{-1} \int_{\partial D(\underline{\lambda}, \varepsilon_0)} (\zeta - T_k(B))^{-1} d\zeta,
$$

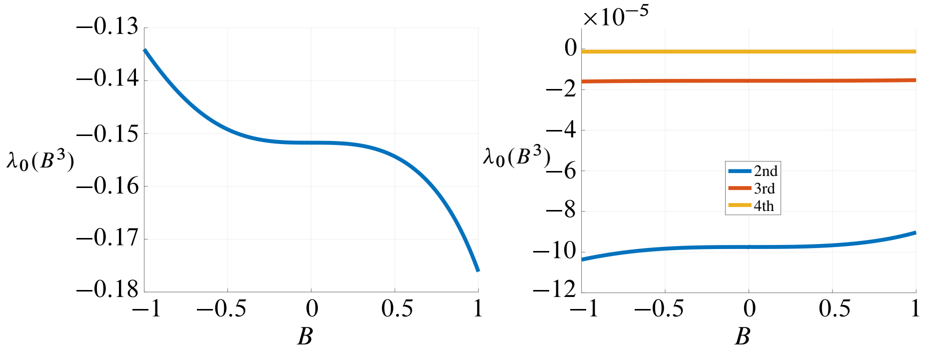

Figure 7. Plot of the $B \mapsto \lambda_1(B)$ of Proposition 5.1 for the first (left) and second-to-fourth magic angles (right).

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 (3.17)), which then implies that the rank is one, and $T_k(B)$ has a simple eigenvalue $\lambda = \lambda(k, B)$. Since

$$\lambda(k, B) = \operatorname{tr}(T_k(B)\Pi(k, B)),$$

it follows that $\lambda(k, B)$ is holomorphic in k and B.

From (2.7) and (5.1), we conclude that

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

This gives

$$\lambda(k, B) = \lambda(-k, B) = \overline{\lambda(\bar{k}, \bar{B})} = \lambda(\omega k, \omega B). \tag{5.6}$$

Definitions (5.2) and (3.6) give $T_{k+p}(B) = \tau(p) T_k(B) \tau(p)^*$, $p \in \Lambda^*$, and hence,

$$\lambda(k + p, B) = \lambda(k, B), \quad p \in \Lambda^* \tag{5.7}$$

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 (5.6):

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

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):

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

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

$$Bk^2 + a_0^{-1}\mu g_1(k,\underline{\alpha}) + \mathcal{O}(\mu^2) + \mathcal{O}(B^2) + \mathcal{O}(Bk^3) = 0, \tag{5.8}$$

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

$$-\mu = \tilde{c}_1 bk^2 + \mathcal{O}(B^3) + \mathcal{O}(Bk^8), \quad \tilde{c}_1 := \underline{\lambda}^{-2} c_1. \tag{5.9}$$

Inserting (5.9) into (5.8) 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), $g_1(0,\underline{\alpha}) \neq 0$. ■

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 $0 \in \mathrm{Spec}_{L^2_0} D_B(\alpha^*)$. Then, the two Bloch eigenvalues $E_{\pm 1}$ of $H^B_k(\alpha)$ closest to zero, defined in (3.16), satisfy

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

Proof. This follows from (4.9) and (5.5). ■

The next proposition deals with the vertices of the boundary of the Brillouin zone. In view of (5.7), it is enough to consider one of the vertices, say,

$$\underline{k}_1 := 2\pi i/\sqrt{3}, \quad z(\underline{k}_1) = \frac{1}{2}. \tag{5.10}$$

We will crucially use the following properties of the theta function defined in (3.23):

$$\theta\left(\frac{1}{2}\right) \neq 0, \quad \theta'\left(\frac{1}{2}\right) = 0, \quad \theta''\left(\frac{1}{2}\right) \neq 0. \tag{5.11}$$

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 the logarithmic derivatives of [12, (2.10b)] or by a rigorous numerical verification based on fast convergence of the sum in (3.23).

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 (5.10),*

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

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:

$$B(k - \underline{k}_1)^2(1 + \mathcal{O}(B)) = c_2^{-1}(1 - \alpha/\underline{\alpha}) - B\lambda_2(B). \tag{5.12}$$

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 (2.7).

Proof of Proposition 5.3. From (5.6), (5.7) and the fact that

$$2k_1 = 4\pi i/\sqrt{3} \in \Lambda^*,$$

we conclude that

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

We also note that, for $k \notin \mathcal{K}_0 + D(0, \varepsilon)$, $\lambda(k, 0) = \underline{\lambda}$ (since $k \in \operatorname{Spec}_{L^2_0} D_0(\alpha)$ only at $\alpha = \underline{\alpha} = 1/\underline{\lambda}$). Hence, as in (5.9) and with the same definition of μ,

$$\begin{aligned} &-\mu = B\lambda_2(B) + \tilde{c}_2 B w^2 + \mathcal{O}(B^2 w^2), \quad w := \underline{k}_1 - k \\ &\tilde{c}_2 := \underline{\lambda}^{-2} c_2, \quad \lambda_2(0) \in \mathbb{R}. \end{aligned} \tag{5.13}$$

We now proceed as in the proof of Proposition 5.1 and use (4.6) and (5.11):

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

This gives the following equation:

$$a_1 B + a_2 B w^2 + a_3 \mu + \mathcal{O}(\mu^2) + \mathcal{O}(B^2) + \mathcal{O}(B w^4) = 0, \quad a_1 a_2 \neq 0. \tag{5.14}$$

Substituting (5.13) into (5.14) shows that $a_3 \neq 0$ and $c_2 \neq 0$. ∎

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:

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

Since $\theta(z(k)) \neq 0$ for $k \notin \Lambda^*$ (see Section 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, [10, Theorem C.8]) for

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

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 $\delta_2 > 0$,

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

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 (2.9): for $U \Subset \mathbb{C}$, for any epsilon, there exits $\rho > 0$ 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 $0 < |B| \le \rho/C$ and $|\alpha - \underline{\alpha}| < \rho|B|/C$ for some (large) constant C.

It remains to prove (2.8). Let F be a fundamental domain of Λ^* containing 0 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,

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

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 (2.9) and putting $K = \{(B, \alpha) : |B| < \delta, \|\alpha - \underline{\alpha}| < a_0\delta|B|\}$, we see that (using [17, Proposition 4.2])

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

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 $k_1 \in \operatorname{Spec} D_B(\alpha) \cap \partial F$, 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 excluding all others from ∂F. The previous argument shows that the number of eigenvalues remains 2. ■

Proof of Theorem 3. When $B, \alpha \in \mathbb{R}$, then the last identity in (2.7) gives

$$\operatorname{Spec}_{L_0^2} D_B(\alpha) = -\operatorname{Spec}_{L_0^2} D_B(\alpha) = \overline{\operatorname{Spec}_{L_0^2} D_B(\alpha)}. \tag{6.2}$$

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

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

(we fix $B \in \mathbb{R}$ here) and (6.2) shows that

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

Since $\overline{\Lambda^*} = \Lambda^*$, this means that $\operatorname{Spec}_{L_0^2} D_B(\alpha) \subset (\mathbb{R} + \Lambda^*) \cup (i\mathbb{R} + \Lambda^*)$ which is the same as (2.10).

To prove (2.11), 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 $\mu = 1/\underline{\alpha} \in \operatorname{Spec}(T_k(0))$. We define $\mathcal{K} := \mathcal{R} \setminus \bigcup_{k' \in \mathcal{K}_0} D(k', \varepsilon)$; then by periodicity of the spectrum of $D_B(\alpha)$, it suffices to restrict us to a fundamental domain: since $\mathcal{K}/\Lambda^*$ 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 $\mu_k \in \operatorname{Spec}(T_k(B))$ 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. ■

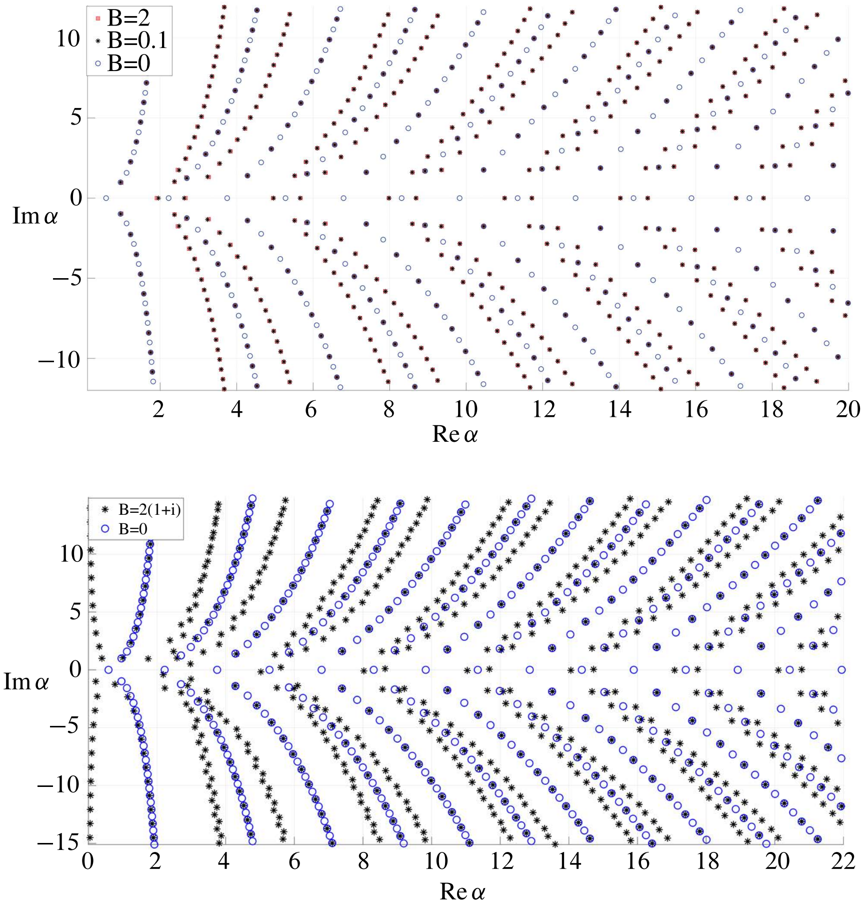

Figure 8. Top figure showing $\alpha \in \mathbb{C}$ such that $1/\alpha \in \operatorname{Spec}_{L^2_0}(T_K(B))$ or $K \in \operatorname{Spec}_{L^2_0}(D_B(\alpha))$. We see that indeed for $B \in \mathbb{R} \setminus \{0\}$ the trajectory of Dirac points passes through K, K'. Bottom figure showing $\alpha \in \mathbb{C}$ such that $1/\alpha \in \operatorname{Spec}_{L^2_0}(T_K(B))$ or $K \in \operatorname{Spec}_{L^2_0}(D_B(\alpha))$. 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.

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 angles, 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.

Acknowledgements. The authors would like to thank Allan MacDonald for suggesting the in-plane magnetic field problem to them, Charles Epstein for a helpful discussion, and the anonymous referee whose detailed comments improved the exposition and led to a correction of a serious mistake.

Funding. MZ was partially supported by the National Science Foundation under Grant DMS-1901462 and by the Simons Foundation Targeted Grant Award no. 896630.

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Received 21 June 2023; revised 14 January 2024.

Simon Becker
ETH Zürich, Institute for Mathematical Research, Rämistrasse 101, 8092 Zurich, Switzerland;
simon.becker@math.ethz.ch

Maciej Zworski
Department of Mathematics, University of California, Berkeley, CA 94720, USA;
zworski@math.berkeley.edu