AN ABSTRACT FORMULATION OF THE FLAT BAND CONDITION

JEFFREY GALKOWSKI AND MACIEJ ZWORSKI

Abstract. Motivated by the study of flat bands in models of twisted bilayer graphene (TBG), we give abstract conditions which guarantee the existence of a discrete set of parameters for which periodic Hamiltonians exhibit flat bands. As an application, we show that a scalar operator derived from the chiral model of TBG has flat bands for a discrete set of parameters.

1. Introduction

Existence of flat bands for periodic operators (in the sense of Floquet theory) has interesting physical consequences, especially in the case of nontrivial band topology. A celebrated recent example is given by the Bistritzer–MacDonald Hamiltonian [BiMa11] modeling twisted bilayer graphene (see [CGG22] and [Wa*22] for its mathematical derivation). A model exhibiting exact flat bands is given by the chiral limit of the Bistritzer–MacDonald model considered by Tarnopolsky–Kruchkov–Vishwanath [TKV19]. Both the Bistritzer–MacDonald model and its chiral limit depend on a parameter corresponding to the angle of twisting between two graphene sheets and, in the chiral model, the perfectly flat bands appear for a discrete set of values of this parameter. This follows from a spectral characterization of those *magic* angles given by Becker–Embree–Wittsten–Zworski [Be*22]. Existence of the first real magic angle was provided by Watson–Luskin [WaLa21], with its simplicity established by Becker–Humbert–Zworski [BHZ22a]. That paper also showed existence of infinitely many, possibly complex, magic angles.

The purpose of this note is to provide a simple abstract version of the spectral characterization of magic angles given in [Be*22] (see also [BHZ22b, Proposition 2.2]). In §3 we apply this spectral characterization of flat bands in a model to which the argument from [Be*22] does not apply.

To formulate our result we consider Banach spaces, $X \subset Y$, and a connected open set $\Omega \subset \mathbb{C}$. The result concerns a holomorphic family of *Fredholm operators of index* 0 (see [DyZw19, §C.2]):

$$Q : \Omega \times \mathbb{C} \to \mathcal{L}(X, Y), \quad (\alpha, k) \mapsto Q(\alpha, k). \tag{1.1}$$

We make the following assumption: there exists a lattice $\Gamma^* \subset \mathbb{C}$, and families of *invertible* operators $\gamma \mapsto W_\bullet(\gamma) : \bullet \to \bullet$, $\bullet = X, Y$, $\gamma \in \Gamma^*$, such that

$$Q(\alpha, k+\gamma) = W_Y(\gamma)^{-1} Q(\alpha, k) W_X(\gamma), \quad \gamma \in \Gamma^*. \tag{1.2}$$

A guiding example is given by the chiral model of twisted bilayer graphene (TBG) [TKV19], [Be*22], [BHZ22b]:

$$\begin{gathered} Q(\alpha, k) := D(\alpha) + k, \quad D(\alpha) := \begin{pmatrix} 2D_{\bar z} & \alpha U(z) \\ \alpha U(-z) & 2D_{\bar z} \end{pmatrix}, \quad \Omega = \mathbb{C}, \\ 2D_{\bar z} = \tfrac{1}{i}(\partial_{x_1} + i\partial_{x_2}), \quad z = x_1 + ix_2 \in \mathbb{C}, \end{gathered} \tag{1.3}$$

where U satisfies

$$\begin{gathered} U(z+\gamma) = e^{i\langle \gamma, K\rangle} U(z), \quad U(\omega z) = \omega U(z), \quad \overline{U(\bar z)} = -U(-z), \quad \omega = e^{2\pi i/3}, \\ \gamma \in \Lambda := \omega \mathbb{Z} \oplus \mathbb{Z}, \quad \omega K \equiv K \not\equiv 0 \mod \Lambda^*, \quad \Lambda^* := \frac{4\pi i}{\sqrt{3}} \Lambda, \quad \langle z, w\rangle := \mathrm{Re}(z\bar w). \end{gathered} \tag{1.4}$$

An example of U is given by the Bistritzer–MacDonald potential

$$U(z) = -\tfrac{4}{3}\pi i \sum_{\ell=0}^{2} \omega^\ell e^{i\langle z, \omega^\ell K\rangle}, \quad K = \tfrac{4}{3}\pi. \tag{1.5}$$

We note that a potential satisfying (1.4) is periodic with respect to the lattice 3Λ and that we can take

$$Y := L^2(\mathbb{C}/\Gamma; \mathbb{C}^2), \quad X := H^1(\mathbb{C}/\Gamma; \mathbb{C}^2), \quad \Gamma := 3\Lambda.$$

(For the Fredholm property of $D(\alpha) + k : X \to Y$ see [Be*22, Proposition 2.3]; the index is equal to 0.) The operators $W_\bullet(\gamma)$ are given by multiplication by $e^{i\langle \gamma, z\rangle}$, $\gamma \in \Gamma^*$, with Γ^* the dual lattice to Γ. (The operator is the same but acts on different spaces.)

The self-adjoint Hamiltonian for the chiral model of TBG is given by

$$H(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* \\ D(\alpha) & 0 \end{pmatrix}, \tag{1.6}$$

and Bloch–Floquet theory means considering the spectrum of

$$\begin{gathered} H_k(\alpha) := e^{-i\langle z, k\rangle} H(\alpha) e^{i\langle z, k\rangle} : H^1(\mathbb{C}/\Gamma; \mathbb{C}^4) \to L^2(\mathbb{C}/\Gamma; \mathbb{C}^4), \\ H_k(\alpha) = \begin{pmatrix} 0 & Q(\alpha, k)^* \\ Q(\alpha, k) & 0 \end{pmatrix}, \quad Q(\alpha, k) = D(\alpha) + k, \end{gathered} \tag{1.7}$$

see [Be*22] (we should stress that it is better to consider a modified boundary condition [BHZ22b] rather than Γ-periodicity but this plays no role in the discussion here).

A *flat band* at zero energy for the Hamiltonian (1.6) means that

$$\begin{aligned} \forall\, k \in \mathbb{C} \ \ 0 \in \mathrm{Spec}_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^4)} H_k(\alpha) \iff & \ \forall\, k \in \mathbb{C} \ \ \ker_{H^1(\mathbb{C}/\Gamma;\mathbb{C}^4)} H_k(\alpha) \neq \{0\} \\ \iff & \ \forall\, k \in \mathbb{C} \ \ \ker_{H^1(\mathbb{C}/\Gamma;\mathbb{C}^2)} Q(\alpha, k) \neq \{0\}. \end{aligned} \tag{1.8}$$

We generalize the result of [Be*22] stating that the set of α's for which (1.8) holds, which we denote by $\mathcal{A}_{\rm ch}$, is a discrete subset of $\mathbb{C}$ and that (1.8) is equivalent to

$$\exists\, k \in \mathbb{C} \setminus \Gamma^* \quad \ker_{H^1(\mathbb{C}/\Gamma;\mathbb{C}^2)} Q(\alpha,k) \neq \{0\}. \tag{1.9}$$

The key property in showing this is the existence of protected states [TKV19], [Be*22]:

$$\forall\, \alpha \in \mathbb{C},\ k \in \Gamma^* \quad \dim\ker_{H^1(\mathbb{C}/\Gamma;\mathbb{C}^2)} Q(k,\alpha) \geq 2, \quad \dim\ker_{H^1(\mathbb{C}/\Gamma;\mathbb{C}^2)} Q(k,0) = 2. \tag{1.10}$$

In the treatment of abstract operators (1.1) we cannot consider the kernel alone as there are many degenerate possibilities – see [DyZw19, §C.4] for a review of the *Gohberg–Sigal* theory relevant to this. In (1.10) semisimplicity of the spectrum of $D(0)$, $Q(k,0) = D(0) + k$ was implicit but this does not need to hold for more general operators, including more general $D(\alpha)$ – see for instance [Ya23]. Hence we will replace (1.10) by a different hypothesis (see (1.13) below) which involves a more general notion of multiplicity: We define multiplicity as follows: if for $\alpha \in \Omega$, there is $k_0 \in \mathbb{C}$ such that $\ker Q(\alpha,k_0) = \{0\}$, then we define

$$m(\alpha,k) := \frac{1}{2\pi i} \operatorname{tr} \oint_{\partial D} Q(\alpha,\zeta)^{-1}\partial_\zeta Q(\alpha,\zeta)d\zeta, \tag{1.11}$$

where the integral is over the positively oriented boundary of a disc D which contains k as the only possible pole of $\zeta \mapsto Q(\alpha,\zeta)$. Otherwise, we put $m(\alpha,k) = \infty$ for all $k \in \mathbb{C}$.

Remarks. 1. Since $k \mapsto Q(\alpha,k)$ is a holomorphic family of Fredholm operators with index 0, we observe that that $\ker Q(\alpha,k_0) = \{0\}$ implies existence of $Q(\alpha,k_0)^{-1}$ and hence $Q(\alpha,\zeta)^{-1}$ is a meromorphic family of operators – see [DyZw19, Theorem C.8]. In particular, (1.11) is well-defined. Hence we have a dichotomy: for a fixed α

$$\forall\, k \quad m(\alpha,k) < \infty \quad \text{or} \quad \forall\, k \quad m(\alpha,k) = \infty. \tag{1.12}$$

2. Assumption (1.2) implies that $m(\alpha,k) = m(\alpha,k+\gamma)$ for any $\gamma \in \Gamma^*$.

3. For any $\alpha \in \Omega$ and $k_1 \in \mathbb{C}$, we have $m(\alpha,k_1) \geq \dim\ker Q(\alpha,k_1)$. If $Q(\alpha,k) = P(\alpha)+k$, $-k_1$ is a semisimple eigenvalue of $P(\alpha)$, and $m(\alpha,k_1) < \infty$, then $m(\alpha,k_1) = \dim\ker Q(\alpha,k_1)$.

Theorem 1. *In the notation of* (1.1) *and assuming* (1.2) *suppose that for some $\alpha_0 \in \Omega$ and every $k \in \mathbb{C}$, we have,*

$$m(\alpha,k) \geq m(\alpha_0,k) \neq \infty. \tag{1.13}$$

Then there exists a discrete set $\mathcal{A} \subset \Omega$ such that for all $k \in \mathbb{C}$

$$m(\alpha,k) = \begin{cases} \infty & \alpha \in \mathcal{A}, \\ m(\alpha_0,k) & \alpha \notin \mathcal{A}. \end{cases} \tag{1.14}$$

In view of (1.10) (and semisimplicity – see Remark 3 above) we see that (1.13) is satisfied for Q given in (1.3) with $\alpha_0 = 0$, $\Omega = \mathbb{C}$ and $m(0,k) = 2\,\mathbb{1}_{\Gamma^*})(k)$. For a direct proof see [Be*22, §3] or [BHZ22b, §2].

Remark. Theorem 1 is valid under a weaker condition than (1.2). As seen in §2, we need to control the multiplicity $m(\alpha,k)$ for every k using $m(\alpha,k)$ for k in some fixed compact set. That some condition is needed (other than holomorphy and the Fredholm property) can be seen by considering the simple example of $Q(\alpha,k) = 1-\alpha k$, $X = Y = \mathbb{C}$. In this case (1.13) is satisfied with $\alpha_0 = 0$ and $m(\alpha_0,k) = 0$. Nevertheless,

$$m(\alpha,k) \geq \dim\ker Q(\alpha,k) = \begin{cases} 0 & k \neq \alpha^{-1} \\ 1 & k = \alpha^{-1} \end{cases}$$

and (1.14) fails. We opted for the easy to state condition (1.2) in view of the motivation from condensed matter physics.

2. Proof of Theorem 1

Define $\mathcal{K} := \operatorname{supp} m(\alpha_0, \bullet)$, which is a discrete set (see Remark 1 above). We now fix $k_0 \in \mathbb{C} \setminus \mathcal{K}$ and define

$$\mathcal{A}_{k_0} := \complement\{\alpha \in \Omega : Q(\alpha,k_0)^{-1} : Y \to X \text{ exists}\}. \tag{2.1}$$

Since $\alpha \mapsto Q(\alpha,k_0)$ is a holomorphic family of Fredholm operators of index zero, and $\ker Q(\alpha_0,k_0) = \{0\}$, we conclude that $\alpha \mapsto Q(\alpha,k_0)^{-1}$ is a meromorphic family of operators and, in particular, $\mathcal{A}_{k_0}$ is a discrete set – see [DyZw19, §C.3]. Also, for $\alpha \notin \mathcal{A}_{k_0}$, $k \mapsto Q(\alpha,k)^{-1}$ is a meromorphic family of operators and hence $m(\alpha,k) < \infty$ for all $k \in \mathbb{C}$ For D as in (1.11), there exists $\varepsilon > 0$ such that

$$m(\alpha,k) = \sum_{k' \in D} m(\alpha',k'), \quad \text{if } |\alpha - \alpha'| < \varepsilon. \tag{2.2}$$

In particular for a fixed $k \in \mathbb{C}$, $\alpha \mapsto m(\alpha,k)$ is upper semicontinuous. We now define

$$U := \{\alpha \in \Omega \setminus \mathcal{A}_{k_0} : \forall\, k,\ m(\alpha,k) = m(\alpha_0,k)\}.$$

We note that $\alpha_0 \in U$ and that $\Omega \setminus \mathcal{A}_{k_0}$ is connected. Hence $U = \Omega \setminus \mathcal{A}_{k_0}$ if we show that U is open and closed in the relative topology of $\Omega \setminus \mathcal{A}_{k_0}$.

Let $\alpha \in U$. We start by showing that for any compact subset $K \subset \mathbb{C}$, there exists $\varepsilon_K > 0$ such that

$$m(\alpha',k) = m(\alpha_0,k) = m(\alpha,k) \text{ for all } k \in K \text{ and } |\alpha - \alpha'| < \varepsilon_K. \tag{2.3}$$

To see this we note that for any fixed $k \in \mathbb{C}$ there exist $D_k = D(k,\delta_k)$, and $\varepsilon_k > 0$ such that that (2.2) holds for $|\alpha - \alpha'| < \varepsilon_k$. By shrinking D_k (and consequently ε_k) we can assume that (here we use the discreteness of $\mathcal{K}$)

$$D_k \setminus \{k\} \subset \complement\mathcal{K}. \tag{2.4}$$

Since K is compact, we can find a finite cover $K \subset \bigcup_{i=1}^{N} D_{k_i}$. Then k_i is the only possible pole for $k \mapsto Q(\alpha, k)^{-1}$ in D_{k_i} and for $|\alpha - \alpha'| < \varepsilon_K := \min_{i=1,\dots N} \varepsilon_{k_i}$, we have

$$m(\alpha, k_i) = \sum_{k \in D_{k_i}} m(\alpha', k),$$

and in particular, as $\alpha \in U$, $m(\alpha_0, k_i) = \sum_{k \in \mathcal{D}_{k_i}} m(\alpha', k)$. Since $m(\alpha', k_i) \geq m(\alpha_0, k_i)$ (by the assumption (1.13)) and $m(\alpha', k) \geq 0$ for all k (since $k \mapsto Q(\alpha, k)$ is holomorphic), we have

$$0 \geq m(\alpha_0, k_i) - m(\alpha', k_i) = \sum_{k \in D_{k_i} \setminus \{k_i\}} m(\alpha', k) \geq 0.$$

Hence, $m(\alpha_0, k_i) = m(\alpha', k_i)$ and $m(\alpha', k) = 0$ for $k \in D_{k_i} \setminus \{k_i\}$. In particular, $m(\alpha', k) = m(\alpha_0, k)$ for all $k \in K$ and $|\alpha' - \alpha| < \varepsilon_K$ as claimed in (2.3).

Now, to complete the proof that U is open, we use (1.2). Let $K \subset \mathbb{C}$ contain the fundamental domain of Γ^* and ε_K as in (2.3). Then, for all $k \in \mathbb{C}$, there is $\gamma \in \Gamma^*$ such that $k + \gamma \in K$. Using (2.3), we have for $|\alpha - \alpha'| < \varepsilon_K$,

$$m(\alpha', k + \gamma) = m(\alpha, k + \gamma).$$

But then, by (1.2) $m(\alpha', k + \gamma) = m(\alpha', k)$, $m(\alpha, k + \gamma) = m(\alpha, k)$, and hence

$$m(\alpha', k) = m(\alpha, k) = m(\alpha_0, k).$$

Since $k \in \mathbb{C}$ was arbitrary, this implies $\alpha' \in U$.

To show that U is closed suppose that $\mathcal{A}_{k_0} \not\ni \alpha_j \to \alpha \notin \mathcal{A}_{k_0}$ and $m(\alpha, k_j) = m(\alpha_0, k)$. Then, since $\alpha \notin \mathcal{A}_{k_0}$, for every $k \in \mathbb{C}$, there exist $\varepsilon_k > 0$ and D_k such that (2.2) and (2.4) hold. In particular, for j large enough (depending on k),

$$m(\alpha, k) = \sum_{k' \in D_k} m(\alpha_j, k') = \sum_{k' \in D_k} m(\alpha_0, k') = m(\alpha_0, k).$$

Hence U is closed and open which means that $U = \Omega \setminus \mathcal{A}_{k_0}$.

Recalling the definition (2.1), we proved that

$$\Omega \setminus \mathcal{A}_{k_0} \subset \{\alpha : \forall\, k,\ m(\alpha, k) = m(\alpha_0, k)\} \subset \Omega \setminus \mathcal{A}_{k_1},$$

for any $k_1 \notin \mathcal{K}$. But this means that $\mathcal{A}_{k_0}$ is independent of k_0 and for $\alpha \in \mathcal{A} := \mathcal{A}_{k_0}$, $Q(\alpha, k)^{-1}$ does not exist for any $k \in \mathbb{C}$. In particular, $m(\alpha, k) = \infty$ for $\alpha \in \mathcal{A}$ and $k \in \mathbb{C}$. $\square$

3. A scalar model for flat bands

One of the difficulties of dealing with the model described by (1.3), (1.6) is the fact that $D(\alpha)$ acts on $\mathbb{C}^2$-valued functions. Here we propose the following model in which

$D(\alpha)$ is replaced by a scalar (albeit second order) operator. This is done as follows. We first consider $P(\alpha) : H^2(\mathbb{C}/\Gamma;\mathbb{C}^2) \to L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)$ defined as follows:

$$\begin{gathered} P(\alpha) := D(-\alpha)D(\alpha) = Q(\alpha)\otimes I_{\mathbb{C}^2} + R(\alpha), \quad Q(\alpha) := (2D_{\bar z})^2 - \alpha^2 V(z), \\ R(\alpha) := -\alpha \begin{pmatrix} 0 & V_1(z) \\ V_1(-z) & 0 \end{pmatrix}, \quad V(z) := U(z)U(-z), \quad V_1(z) := 2D_{\bar z}U(z). \end{gathered} \tag{3.1}$$

If we think of $P(\alpha)$ as a semiclassical differential system with $h = 1/\alpha$ (see [DyZw19, §E.1.1]) then $Q(\alpha)$ is the quantization of the determinant of the symbol of $D(\alpha)$ and $R(\alpha)$ is a lower order term. We lose no information when considering $P(\alpha)$ in the characterization of flat bands (1.8):

Proposition 1. *If $P(\alpha,k) := e^{-i\langle z,k\rangle}P(\alpha)e^{i\langle z,k\rangle}$ then*

$$\ker_{H^1(\mathbb{C}/\Gamma)}(D(\alpha)+k) \neq \{0\} \iff \ker_{H^2(\mathbb{C}/\Gamma)} P(\alpha,k) \neq \{0\}. \tag{3.2}$$

In particular $\alpha \in \mathcal{A}_{\rm ch}$ if and only if $k \in \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)} P(\alpha,k)$ for some $k \notin \Gamma^*$ (which then implies this for all k).

Proof. We note that $P(\alpha,k) = (D(-\alpha)+k)(D(\alpha)+k)$ and that

$$D(-\alpha) - k = -\mathscr{R}(D(\alpha)+k)\mathscr{R}, \quad \mathscr{R}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}(z) = \begin{pmatrix} u_2(-z) \\ u_1(-z) \end{pmatrix}$$

and hence

$$\ker_{H^1(\mathbb{C}/\Gamma)}(D(\alpha)+k) = \mathscr{R}\ker_{H^1(\mathbb{C}/\Gamma)}(D(-\alpha)-k).$$

Since $D(\alpha)$ is elliptic, the elements of the kernels above are in $C^\infty(\mathbb{C}/\Gamma)$ and hence H^1 can be replaced by H^s for any s – see [DyZw19, Theorem 3.33]. Hence if $\ker_{H^2} P(\alpha,k) \neq \{0\}$ then either $\ker_{H^2}(D(\alpha)+k) = \ker_{H^1}(D(\alpha)+k) \neq \{0\}$ or $\ker_{H^1}(D(-\alpha)+k) \neq \{0\}$. If $k \notin \Gamma^*$ then the equivalence of (1.9) and (1.8) gives the conclusion. ☐

We now consider a model in which we drop the matrix terms in (1.1), the definition of $P(\alpha)$, and have $Q(\alpha)$ act on scalar valued functions. The self-adjoint Hamiltonian corresponding to (1.6) is now given by

$$\begin{gathered} H(\alpha) := \begin{pmatrix} 0 & Q(\alpha)^* \\ Q(\alpha) & 0 \end{pmatrix}, \quad Q(\alpha) := (2D_{\bar z})^2 - \alpha^2 V(z), \quad V \in C^\infty(\mathbb{C}), \\ V(x+\gamma) = V(x), \quad \gamma \in \Lambda := \omega\mathbb{Z}\oplus\mathbb{Z}, \quad V(\omega x) = \bar\omega V(x), \quad \omega := e^{2\pi i/3}. \end{gathered} \tag{3.3}$$

The potential is periodic with respect to Λ, and hence the usual Floquet theory applies:

$$\begin{gathered} H(\alpha,k) := \begin{pmatrix} 0 & Q(\alpha,k)^* \\ Q(\alpha,k) & 0 \end{pmatrix}, \quad Q(\alpha,k) := (2D_{\bar z}+k)^2 - \alpha^2 V(z), \\ \operatorname{Spec}_{L^2(\mathbb{C})} H(\alpha) = \bigcup_{k\in\mathbb{C}/\Lambda^*} \operatorname{Spec}_{L^2(\mathbb{C}/\Lambda)} H(\alpha,k), \end{gathered} \tag{3.4}$$

where $\mathrm{Spec}_{L^2(\mathbb{C}/\Lambda)} H(\alpha,k)$ is discrete and is symmetric under $E \mapsto -E$. Just as for the chiral model of TBG, a flat band at zero for a given α means that

$$\forall\, k \in \mathbb{C} \;\; 0 \in \mathrm{Spec}_{L^2(\mathbb{C}/\Lambda;\mathbb{C}^2)} H(\alpha,k) \iff \forall\, k \in \mathbb{C} \;\; \ker_{H^2(\mathbb{C}/\Lambda;\mathbb{C})} Q(\alpha,k) \neq \{0\}.$$

As in the chiral model, we take $W_X(\gamma) = W_Y(\gamma) = e^{i\langle \gamma, z\rangle}$, $\gamma \in \Lambda^*$, the dual lattice to obtain (1.2). Theorem 1 shows that as in the case of (1.6) this happens for a discrete set of $\alpha \in \mathbb{C}$:

Theorem 2. *For H and Q given in (3.3) there exists a discrete set $\mathcal{A}_{\rm sc} \subset \mathbb{C}$ such that*

$$\begin{gathered} \ker_{H^2(\mathbb{C}/\Lambda;\mathbb{C})} Q(\alpha,k) \neq \{0\} \quad \textit{for } \alpha \in \mathcal{A}_{\rm sc},\ k \in \mathbb{C}, \\ m(\alpha,k) = 2\,\mathbb{1}_{\Lambda^*}(k) \quad \textit{for } \alpha \notin \mathcal{A}_{\rm sc}. \end{gathered} \tag{3.5}$$

This is an immediate consequence of Theorem 2 once we establish (1.13) with $m(0,k) = 2\,\mathbb{1}_{\Lambda^*}(k)$ (i.e. $\alpha_0 = 0$). The kernel of $Q(0,k) = 2(D_{\bar z} + k)^2$, on $H^2(\mathbb{C}/\Lambda)$ is empty for $k \notin \Lambda^*$ and is given by $\mathbb{C}e^{i\langle k,z\rangle}$, when $k \in \Lambda^*$. This gives that $m(0,k) = 2\,\mathbb{1}_{\Lambda^*}(k)$ after noticing that $D_{\bar z}$ is diagonal in the basis $\{e^{i\langle k,z\rangle}\}_{k\in\Lambda^*}$ of $H^2(\mathbb{C}/\Lambda;\mathbb{C})$ and $\partial_k (D_{\bar z} + k)^2|_{k=k_0} e^{i\langle k_0,z\rangle} = 0$ for $k_0 \in \Lambda^*$. The second one is provided by

Proposition 2. *For all $\alpha \in \mathbb{C}$ and $k \in \Lambda^*$, $m(\alpha,k) \geq 2$.*

Proof. The proof uses the symmetry of $Q(\alpha,k)$ under the action $k \mapsto \omega k$ in a way similar to its use in [BZ23a] and [Be*23].

We first recall that (1.2) implies that $m(\alpha, k+\gamma) = m(\alpha,k)$ for $\gamma \in \Gamma^*$ and hence it is enough to show that $m(\alpha,0) \geq 2$ for all α. We then define

$$\mathcal{C} := \{\alpha \in \mathbb{C} \,:\, m(\alpha,k) < \infty, \;\text{ for all } k \in \mathbb{C}\} = \{\alpha \,:\, m(\alpha,k_0) < \infty\},$$

where the second equality holds, in view of (1.12), for any $k_0 \in \mathbb{C}$. This set is connected, as for $k_0 \notin \Lambda^*$, $Q(\alpha,k_0)^{-1}$ exists and hence $\alpha \mapsto Q(\alpha,k_0)^{-1}$ is a meromorphic family of operators (we use [DyZw19, Theorem C.8] again).

Next, we observe that,

$$Q(\alpha,k)\Omega = \omega\Omega Q(\alpha,\omega k), \quad \Omega u(z) := u(\omega z),$$

and that gives, for $\alpha \in \mathcal{C}$,

$$m(\alpha,k) = m(\alpha,\omega k) = m(\alpha,\omega^2 k). \tag{3.6}$$

We now let

$$\mathcal{B} := \{\alpha \in \mathcal{C} \,:\, m(\alpha,0) = 2 \mod 3\}.$$

and claim that $\mathcal{B} = \mathcal{C}$. This will finish the proof since $m(\alpha,k) \geq 0$ implies that $\mathcal{B} \subset \{\alpha \in \mathcal{C} \,:\, m(\alpha,0) \geq 2\}$. Since $0 \in \mathcal{B}$ and $\mathcal{C}$ is connected, to show that $\mathcal{B} = \mathcal{C}$, it is enough to show that $\mathcal{B} \subset \mathcal{C}$ is open and closed in the relative topology of $\mathcal{C}$.

We start by showing that $\mathcal{B}$ is open and for that choose $\alpha_0 \in \mathcal{B}$. Then, in view of (2.2) and (3.6), there exists a disk, D, around 0 and $\varepsilon > 0$ such that for $|\alpha - \alpha_0| < \varepsilon$,

$$\begin{aligned} 2 = m(\alpha_0, 0) &= \sum_{k \in D} m(\alpha, k) = m(\alpha, 0) + \sum_{k \in D \setminus \{0\}} m(\alpha, k) \\ &= m(\alpha, 0) + 3 \sum_{\substack{k \in D \setminus \{0\} \\ 0 \leq \arg k < \frac{2\pi}{3}}} m(\alpha, k). \end{aligned}$$

It follows that $m(\alpha, 0) = 2 \bmod 3$ which implies that $\alpha \in \mathcal{B}$ for $|\alpha - \alpha_0| < \varepsilon$, that is, $\mathcal{B}$ is open as claimed.

Next, we show $\mathcal{B}$ is closed. To see this, suppose that $\alpha_j \in \mathcal{B}$ with $\alpha_j \to \alpha \in \mathcal{C}$. Then, for j large enough, (2.2) gives

$$m(\alpha, 0) = \sum_{k \in D} m(\alpha_j, k) = m(\alpha_j, 0) + \sum_{k \in D \setminus \{0\}} m(\alpha_j, k) = 2 + 3 \sum_{\substack{k \in D \setminus \{0\} \\ 0 \leq \arg k < \frac{2\pi}{3}}} m(\alpha_j, k).$$

Hence, $m(\alpha, 0) = 2 \bmod 3$, that is $\mathcal{B}$ is closed. $\square$

Remarks. 1. The proof of Theorem 1 also shows the following spectral characterization of $\mathcal{A}_{\mathrm{sc}}$: if

$$T_k := (2D_{\bar{z}} + k)^{-2} V, \quad k \notin \Lambda^*, \tag{3.7}$$

then

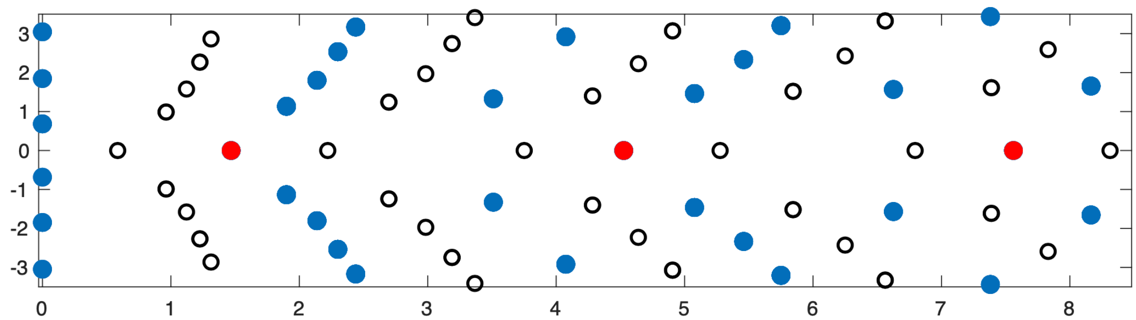
$$\begin{aligned} \alpha \in \mathcal{A}_{\mathrm{sc}} &\iff \exists\, k \notin \Lambda^* \quad \alpha^{-2} \in \operatorname{Spec}_{L^2(\mathbb{C}/\Lambda)} T_k \\ &\iff \forall\, k \notin \Lambda^* \quad \alpha^{-2} \in \operatorname{Spec}_{L^2(\mathbb{C}/\Lambda)} T_k, \end{aligned} \tag{3.8}$$

Using the methods of [BHZ22a] one can show that for $V(z) = U(z)U(-z)$ with U given by (1.5) (or for more general classes of potentials described in [BHZ22a]), $\operatorname{tr} T_k^p \in (\pi/\sqrt{3})\mathbb{Q}$, $p \geq 2$. Together with a calculation for $p = 2$ (as in [Be*22]) this shows that $|\mathcal{A}_{\mathrm{sc}}| = \infty$. With numerical assistance one can also show existence of a real $\alpha \in \mathcal{A}_{\mathrm{sc}}$.

2. We can strengthen Proposition 2 as in [BHZ22b, Proposition 2.3]: there exists a holomorphic family $\mathbb{C} \ni \alpha \mapsto u(\alpha) \not\equiv 0$, such that $u(0) = 1$ and $Q(\alpha, 0)u(\alpha) = 0$.

4. Numerical observations

The spectral characterization (3.8) allows for an accurate computation of α's for which (3.3) exhibits flat bands at energy 0. For large α's however, pseudospectral effects described in [Be*22] make calculations unreliable. The set (shown as $\bullet$) $\mathcal{A}_{\mathrm{sc}} \cap \{\operatorname{Re} \alpha \geq 0\}$ where $\mathcal{A}_{\mathrm{sc}}$ is given in Theorem 2 looks as follows (for comparison we show the corresponding set, $\mathcal{A}_{\mathrm{ch}}$, for the chiral model $\circ$):



The real elements of $\mathcal{A}_{\mathrm{sc}}$ are shown as $\color{red}\bullet$. They appear to have multiplicity two. An adaptation of the theta function argument [DuNo80], [TKV19], [Be*22], [BHZ22b, §3.2] should apply to this case and the evenness of eigenfunctions in Proposition 2 shows that they have (at least) two zeros at $\alpha \in \mathcal{A}_{\mathrm{sc}}$. That implies multiplicity of at least 2. This is illustrated by an animation `https://math.berkeley.edu/~zworski/scalar_magic.mp4` (shown in the coordinates of [Be*22]). When we interpolate between the chiral model and the scalar model, the multiplicity two real α's split and travel in opposite directions to become magic α's for the chiral model: see `https://math.berkeley.edu/~zworski/Spec.mp4`.

One of the most striking observations made in [TKV19] was a quantization rule for real elements of $\mathcal{A}_{\mathrm{ch}}$ with the exact potential (1.4): if $\alpha_1 < \alpha_2 < \cdots \alpha_j < \cdots$ is the sequence of all real α's for which (1.8) holds, then

$$\alpha_{j+1} - \alpha_j = \gamma + o(1), \quad j \to +\infty, \quad \gamma \simeq \tfrac{3}{2}. \tag{4.1}$$

The more accurate computations made in [Be*22] suggests that $\gamma \simeq 1.515$.

In the scalar model (3.3) with $V(z) = U(z)U(-z)$ where U is given by (1.4) we numerically observe the following rule for real elements of $\mathcal{A}_{\mathrm{sc}}$:

$$\alpha_{j+1} - \alpha_j = 2\gamma + o(1), \quad j \to +\infty, \tag{4.2}$$

where γ is the same as in (4.1).

Acknowledgements. We would like to thank Simon Becker for help with matlab and in particular for producing the movies referred to above. JG acknowledges support from EPSRC grants EP/V001760/1 and EP/V051636/1 and MZ from the NSF grant DMS-1901462 and the Simons Foundation under a "Moiré Materials Magic" grant.

References

[Be*23] S. Becker, T. Humbert, J. Wittsten and M. Yang, *Chiral limit of twisted trilayer graphene*, arXiv:2308.10859.

[Be*21] S. Becker, M. Embree, J. Wittsten and M. Zworski, *Spectral characterization of magic angles in twisted bilayer graphene,* Phys. Rev. B **103**, 165113, 2021.

[Be*22] S. Becker, M. Embree, J. Wittsten and M. Zworski, *Mathematics of magic angles in a model of twisted bilayer graphene*, Probab. Math. Phys. **3**(2022), 69–103.

[BHZ22a] S. Becker, T. Humbert and M. Zworski, *Integrability in the chiral model of magic angles*, arXiv:2208.01620.

[BHZ22b] S. Becker, T. Humbert and M. Zworski, *Fine structure of flat bands in a chiral model of magic angles,* arXiv:2208.01628.

[BZ23a] S. Becker and M. Zworski, *Dirac points for twisted bilayer graphene with in-plane magnetic field*, arXiv:2303.00743.

[BiMa11] R. Bistritzer and A. MacDonald, *Moiré bands in twisted double-layer graphene.* PNAS, **108**, 12233–12237, 2011.

[CGG22] E. Cancès, L. Garrigue, D. Gontier, *A simple derivation of moiré-scale continuous models for twisted bilayer graphene.* arXiv:2206.05685.

[DuNo80] B.A. Dubrovin and S.P. Novikov, *Ground states in a periodic field. Magnetic Bloch functions and vector bundles.* Soviet Math. Dokl. **22**, 1, 240–244, 1980.

[DyZw19] S. Dyatlov and M. Zworski, *Mathematical Theory of Scattering Resonances,* AMS 2019, `http://math.mit.edu/~dyatlov/res/`

[TKV19] G. Tarnopolsky, A.J. Kruchkov and A. Vishwanath, *Origin of magic angles in twisted bilayer graphene*, Phys. Rev. Lett. 122, 106405, 2019

[Wa*22] A. B. Watson, T. Kong, A. H. MacDonald, and M. Luskin, *Bistritzer-MacDonald dynamics in twisted bilayer graphene*, arXiv:2207.13767.

[WaLa21] A. Watson and M. Luskin, *Existence of the first magic angle for the chiral model of bilayer graphene*, J. Math. Phys. **62**, 091502 (2021).

[Ya23] M. Yang, *Flat bands and high Chern numbers in twisted multilayer graphene,* arXiv:2303.00103.

Email address: j.galkowski@ucl.ac.uk

Department of Mathematics, University College London, WC1H 0AY, UK

Email address: zworski@math.berkeley.edu

Department of Mathematics, University of California, Berkeley, CA 94720