MATHEMATICS OF MAGIC ANGLES IN A MODEL OF TWISTED BILAYER GRAPHENE

SIMON BECKER, MARK EMBREE, JENS WITTSTEN, AND MACIEJ ZWORSKI

Abstract. We provide a mathematical account of the recent Physical Reviews Letter by Tarnopolsky–Kruchkov–Vishwanath [TKV19]. The new contributions are a spectral characterization of magic angles, its accurate numerical implementation and an exponential estimate on the squeezing of all bands as the angle decreases. Pseudospectral phenomena [DSZ04],[TrEm05], due to the non-hermitian nature of operators appearing in the model considered in [TKV19] play a crucial role in our analysis.

1. Introduction and statement of results

Following a recent Physical Review Letter by Tarnopolsky–Kruchkov–Vishwanath [TKV19] we consider the following Hamiltonian modeling twisted bilayer graphene:

$$H(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* \\ D(\alpha) & 0 \end{pmatrix}, \quad D(\alpha) := \begin{pmatrix} 2D_{\bar z} & \alpha U(z) \\ \alpha U(-z) & 2D_{\bar z} \end{pmatrix}, \tag{1.1}$$

where $z = x_1 + ix_2$, $D_{\bar z} := \frac{1}{2i}(\partial_{x_1} + i\partial_{x_2})$ and

$$U(z) = U(z, \bar z) := \sum_{k=0}^{2} \omega^k e^{\frac12 (z\bar\omega^k - \bar z \omega^k)}, \quad \omega := e^{2\pi i/3}. \tag{1.2}$$

(We abuse the notation in the argument of U for the sake of brevity and write $U(z)$ rather than $U(z, \bar z)$.) The dimensionless parameter α is essentially the reciprocal of the

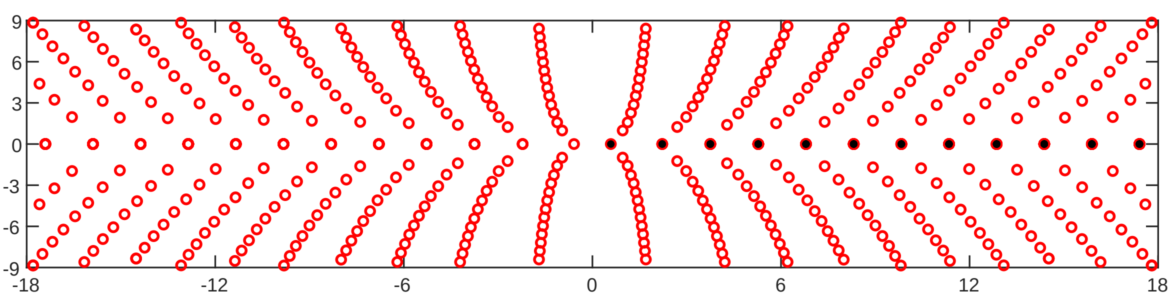

Figure 1. Reciprocals of magic angles for the specific potential (1.2): resonant α's (red circles) come from the full spectrum of the compact operator (1.9) defining magic angles, and the magic α's (black dots) are the reciprocals of the "physically relevant" positive angles.

angle of twisting between the two layers. When two honeycomb lattices are twisted against one another, a periodic honeycomb superlattice, called the moiré lattice, becomes visible. (This name comes from the patterns formed when two fabrics lie on top of each other.) Bistritzer and MacDonald in [BiMa11] predicted that the symmetries of the periodic moiré lattice lead to dramatic flattening of the band spectrum. The operator (1.1) and in particular potential (1.2) were obtained in [TKV19] by removing certain interaction terms from the operator constructed in [BiMa11].

In this paper we consider any potential having the symmetries of (1.2):

$$\begin{gathered} \mathbf{a} = \tfrac{4}{3}\pi i \omega^\ell, \ \ \ell = 1,2 \implies U(z+\mathbf{a}) = \bar{\omega} U(z), \ \text{and} \\ U(\omega z) = \omega U(z). \end{gathered} \tag{1.3}$$

The only exception is Theorem 4 which requires a non-triviality assumption, see (4.3). Such potentials are explored further in Section 4.

The Hamiltonian H is periodic with respect to a lattice Γ (see (2.2) below) and *magic angles* are defined as the α's (or rather their reciprocals) at which

$$0 \in \bigcap_{\mathbf{k}\in\mathbb{C}} \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_{\mathbf{k}}(\alpha)), \quad H_{\mathbf{k}}(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* - \bar{\mathbf{k}} \\ D(\alpha) - \mathbf{k} & 0 \end{pmatrix}. \tag{1.4}$$

The Hamiltonian $H_{\mathbf{k}}(\alpha)$ comes from the *Floquet theory* of $H(\alpha)$ and (1.4) means that $H(\alpha)$ has a *flat band* at 0 (see Proposition 2.4 below). Since the Bloch electrons have the same energy at the flat bands, strong electron-electron interactions leading to effects such as superconductivity have been observed at magic angles. We refer to [TKV19] for physical motivation and references. Some aspects of this paper carry over to more general models such as the Bistritzer–MacDonald [BiMa11] and that is discussed in [B*21].

The first theorem is, essentially, the main mathematical result of [TKV19]. To formulate it we define the Wronskian of two $\mathbb{C}^2$-valued Γ-periodic functions:

$$W(\mathbf{u},\mathbf{v}) = \det[\mathbf{u},\mathbf{v}], \quad \mathbf{u},\mathbf{v} \in \mathbb{C}^2, \tag{1.5}$$

noting that if $D(\alpha)\mathbf{u} = D(\alpha)\mathbf{v} = 0$, then W is constant (applying $\partial_{\bar z}$ shows that W is holomorphic and periodic). We also define an involution $\mathscr{E}$ satisfying $\mathscr{E} D(\alpha) = D(\alpha)\mathscr{E}$:

$$\mathscr{E}\mathbf{u}(\alpha,z) := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathbf{u}(\alpha,-z). \tag{1.6}$$

We then have

Theorem 1. *Suppose that $D(\alpha)$ is given by (1.1) with $U \in C^\infty(\mathbb{C}/\Gamma;\mathbb{C})$ satisfying (1.3). Then there exists a real-analytic function f on $\mathbb{R}$ such that*

$$0 \in \bigcap_{\mathbf{k}\in\mathbb{C}} \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_{\mathbf{k}}(\alpha)) \iff f(\alpha) = 0.$$

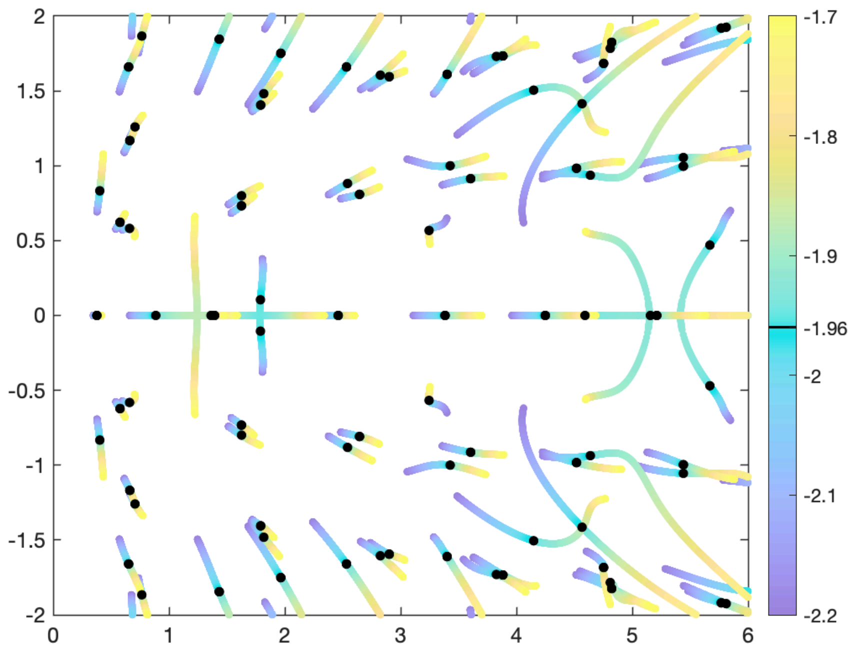

FIGURE 2. For $U_\mu(z) = U(z) + \mu \sum_{k=0}^{2} \omega^k e^{\bar z \omega^k - z \bar\omega^k}$, with U given by (1.2) and $\mu = -1.96$, we show set $\mathcal{A}$ (indicated by $\bullet$). The distribution is much less regular than for $\mu = 0$ shown in Figure 1, and nothing like (1.12) can be expected. The coloured paths trace the dynamics of magic α's for $-2.2 \le \mu \le -1.7$: to understand the dependence of "physically relevant" real α's complex values should be considered.

The function f is defined using a projectively unique family $\mathbb{R} \ni \alpha \mapsto \mathbf{u}(\alpha) \in C^\infty(\mathbb{C}/\Gamma; \mathbb{C}^2)$ such that $\mathbf{u}(0) = (1,0)^t$, $D(\alpha)\mathbf{u}(\alpha) = 0$. Then $f(\alpha) := W(\mathbf{u}(\alpha), \mathscr{E}\mathbf{u}(\alpha))$, where W is given by (1.5) *and $\mathscr{E}$ is defined in* (1.6).

A more precise, representation theoretical, description of $\mathbf{u}(\alpha)$ will be given in §2. Projective uniqueness means uniqueness up to a multiplicative factor. In §3 we show that (after possibly switching $\mathbf{u}$ and $\mathscr{E}\mathbf{u}$)

$$v(\alpha) := W(\mathbf{u}(\alpha), \mathscr{E}\mathbf{u}(\alpha)) = 0 \iff \mathbf{u}(\alpha, z_S) = 0, \quad z_S := \tfrac{4\sqrt{3}}{9}\pi, \tag{1.7}$$

which then provides a recipe [TKV19] for constructing the zero eigenfunctions of $H_{\mathbf{k}}(\alpha)$: if $v(\alpha) = 0$ then $(D(\alpha) - \mathbf{k})\mathbf{u}_{\mathbf{k}}(\alpha) = 0$, $\mathbf{u}_{\mathbf{k}}(\alpha) \in C^\infty(\mathbb{C}/\Gamma; \mathbb{C}^2)$, where

$$\mathbf{u}_{\mathbf{k}}(z) = e^{\frac{i}{2}(z\bar{\mathbf{k}} + \bar z \mathbf{k})} \frac{\theta_{-\frac16 + k_1/3, \frac16 - k_2/3}(3z/4\pi i\omega|\omega)}{\theta_{-\frac16, +\frac16}(3z/4\pi i\omega|\omega)} \mathbf{u}(z), \quad \mathbf{k} = \tfrac{1}{\sqrt3}(k_1\omega^2 - k_2\omega), \tag{1.8}$$

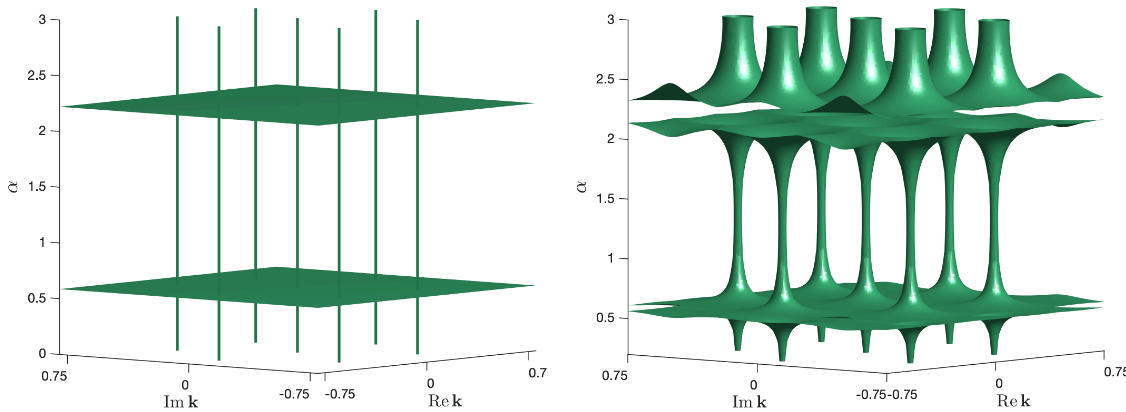

FIGURE 3. Left: spectrum of $D(\alpha)$ as α varies. Right: level surface of $\mathbf{k} \mapsto \|(D(\alpha)-\mathbf{k})^{-1}\| = 10^2$ as α varies: we see that the norm of the resolvent $(D(\alpha)-\mathbf{k})^{-1}$ grows as we approach the first two magic α's (near 0.586 and 2.221), at which it blows up for all k. In any discretization that norm would be finite except on a finite set but it would blow up as the discretization improves.

where $\zeta \mapsto \theta_{a,b}(\zeta|\omega)$ is the Jacobi theta function – see §3.2 for a brief review and [Mu83, Chapter I] for a proper introduction. (Our convention is slightly different than that in [TKV19] but the formulas are equivalent.)

The next theorem provides a simple spectral characterization of α's satisfying (1.4). Combined with some symmetry reductions (see §§2,5) this characterization allows a precise calculation of the leading magic α's – see Table 1 for the values of the first 13 elements of $\mathcal{A}_{\rm mag}$ and Tables 2, 3 for rigorous error bounds. As seen in Proposition 5.2, it also implies that the multiplicities of flat bands at 0 is at least 18.

Theorem 2. *Let Γ^* be the dual lattice and define the family of compact operators*

$$T_{\mathbf{k}} := (2D_{\bar z} - \mathbf{k})^{-1} \begin{pmatrix} 0 & U(z) \\ U(-z) & 0 \end{pmatrix}, \quad \mathbf{k} \notin \Gamma^*, \tag{1.9}$$

where $U(z)$ is given by (1.2), or more generally satisfies $U \in C^\infty(\mathbb{C}/\Gamma;\mathbb{C})$ and (1.3). Then the spectrum of $T_{\mathbf{k}}$ is independent *of $\mathbf{k} \notin \Gamma^*$, and the following statements are equivalent:*

1. $1/\alpha \in \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(T_{\mathbf{k}})$, $\quad \mathbf{k} \notin \Gamma^*$;
2. $\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \mathbb{C}$;
3. $0 \in \bigcap_{\mathbf{k}\in\mathbb{C}} \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_{\mathbf{k}}(\alpha))$, *where $H_{\mathbf{k}}$ is defined in (1.4).*

We denote the full set of *resonant* α's and the set of *magic* α's as

$$\begin{aligned} \mathcal{A} &:= 1/(\mathrm{Spec}_{L^2(\mathbb{C}/\Gamma)}(T_{\mathbf{k}}) \setminus \{0\}), \quad \mathbf{k} \notin \Gamma^*, \\ \mathcal{A}_{\mathrm{mag}} &:= \mathcal{A} \cap (0,\infty) = \{\alpha_j\}_{j\geq 1}, \quad \alpha_1 < \alpha_2 < \cdots , \end{aligned} \tag{1.10}$$

respectively. The elements of $\mathcal{A}$ are *included with their multiplicities* as multiplicities of eigenvalues of $T_{\mathbf{k}}$. Those multiplicities are at least 9 – see Proposition 5.2. Numerical evidence suggests that multiplicities of $\mathcal{A}_{\mathrm{mag}}$ are exactly 9 and that is related to the question about zeros of $u(\alpha)$ – see (1.7) and Remark 1 after Proof of Theorem 1 in §3.

As a simple byproduct of Theorems 1 and 2 we have

$$\mathrm{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \Gamma^*, \quad \alpha \notin \mathcal{A}.$$

Examples of operators which have either discrete spectra or all of $\mathbb{C}$ as spectrum, depending on analytic variation of coefficients, have been known before, see for instance Seeley [Se86]. The operator $D(\alpha)$ provides a new striking example of such phenomena, showing that it is physically relevant and not merely pathological.

If we assume that $U(z) = \overline{U(\bar{z})}$, then Proposition 3.2 below (see also Figure 1) also gives $\mathcal{A} = -\mathcal{A} = \overline{\mathcal{A}}$.

Mathematical description of $\mathcal{A}$ remains open and here we only contribute the following simple result:

Theorem 3. *For the potential U given by (1.2) we have*

$$\sum_{\alpha\in\mathcal{A}} \alpha^{-4} = 72\pi/\sqrt{3}, \tag{1.11}$$

where α's are included according to their multiplicities. In particular, $\mathcal{A} \neq \emptyset$.

Concerning $\mathcal{A}_{\mathrm{mag}}$, an intriguing asymptotic relation for α_j's for U given by (1.2) was suggested by the numerics in [TKV19]:

$$\alpha_{j+1} - \alpha_j \simeq \tfrac{3}{2}, \quad j \gg 1. \tag{1.12}$$

We do not address this problem here except numerically in §5 and in Figure 2, which shows that regular spacing does not hold for general potentials. The following result based on Dencker–Sjöstrand–Zworski [DSZ04] indicates the mathematical subtlety underlying the distribution problem: for large values of α the bands get exponentially squeezed, making it difficult to find the ones that are exactly zero; see Figure 4 and the following

Theorem 4. *Suppose that $H_{\mathbf{k}}(\alpha)$ is given by (1.1) and (1.4) with U given by (1.2) and that*

$$\mathrm{Spec}_{L^2(\mathbb{C}/\Gamma)} H_{\mathbf{k}}(\alpha) = \{E_j(\mathbf{k},\alpha)\}_{j\in\mathbb{Z}}, \quad E_j(\mathbf{k},\alpha) \leq E_{j+1}(\mathbf{k},\alpha), \quad \mathbf{k}\in\mathbb{C}, \quad \alpha > 0,$$

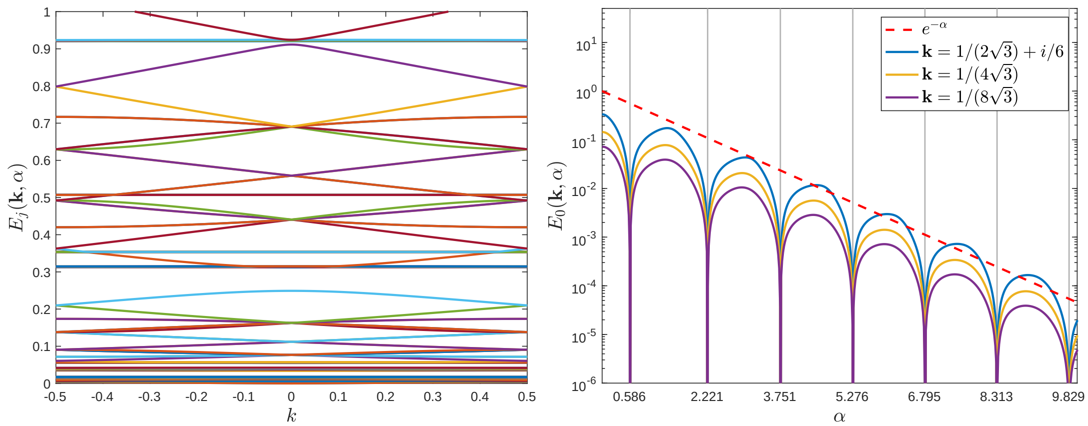

FIGURE 4. On the left, the smallest non-negative eigenvalues of $H_{\mathbf{k}}(\alpha)$, $\alpha=5$, $\mathbf{k}=k\omega/\sqrt{3}$, $-\frac{1}{2}\leq k\leq\frac{1}{2}$. On the right, $E_0(\mathbf{k},\alpha)$ (log scale) for several values $\mathbf{k}$. (The point $\mathbf{k}=1/(2\sqrt{3})+i/6$ is farthest from an eigenvalue of $D(\alpha)$ for $\alpha\notin\mathcal{A}$.) The exponential squeezing of the bands described in Theorem 4 is clearly visible.

with the convention that $E_0(\mathbf{k},\alpha)=\min_j|E_j(\mathbf{k},\alpha)|$. *Then there exist positive constants* c_0, c_1, *and* c_2 *such that for all* $\mathbf{k}\in\mathbb{C}$,

$$|E_j(\mathbf{k},\alpha)|\leq c_0e^{-c_1\alpha},\quad |j|\leq c_2\alpha,\quad \alpha>0. \tag{1.13}$$

Numerical experiments presented in Figure 7 (see also Figure 4) suggest that for any c_2 there exists c_0 for which (1.13) holds, with $c_1=1$. The theorem is proved by showing that for large α every point "wants to be" in the spectrum of $D(\alpha)$ modulo an exponentially small error. That is a typical *pseudospectral* effect in the study of non-hermitian operators – see Trefethen–Embree [TrEm05] for a broad description of such phenomena. Although $H_{\mathbf{k}}(\alpha)$ is self-adjoint, having a zero eigenvalue is equivalent to $\mathbf{k}\in\mathrm{Spec}_{L^2(\mathbb{C}/\Gamma)}(D(\alpha))$ and $D(\alpha)$ is highly non-normal. This is illustrated in Figure 3. In Section 4 we explore the situation for general potentials satisfying the symmetries (1.3), and prove that a result corresponding to Theorem 4 continues to hold if an additional non-triviality assumption is imposed; see (4.3) and Theorem 5. (Some condition is clearly needed, as shown by the example of $U\equiv 0$.)

Watson and Luskin [WaLu21] have recently provided an alternative proof of Theorem 1 and implemented it numerically with precise error bounds. Assuming accuracy of singular value and polynomial calculations they proved existence of $\alpha_1\in\mathcal{A}_{\mathrm{mag}}$, $\alpha_1\simeq 0.586$. Motivated by [WaLu21] we added error estimates for our calculations in §5.2. Assuming accuracy of singular value estimates for large sparse matrices we show existence of α_1 within 10^{-9} and α_2 within 10^{-3} – see Tables 2 and 3. However, we do have high confidence in all digits shown in Table 1.

2. Hamiltonian and its symmetries

In this section we discuss symmetries of $D(\alpha)$ and $H(\alpha)$ and prove basic results about their spectra.

Before entering mathematical analysis of the model we provide a brief motivation for the Hamiltonian. Two basic symmetries are inherited from the honeycomb structure of the moiré lattice: a translation symmetry and a rotational symmetry by $2\pi/3$. In addition, the model exhibits a chiral symmetry which accounts for the massless and symmetric Dirac cones of the model that are preserved by the tunneling interaction. The Dirac cones are effectively described by $2D$-massless Dirac operators. Therefore, the cones of two non-interacting sheets of graphene are described by a kinetic Hamiltonian

$$H_{\rm kin} = \operatorname{diag}(H_{\rm Dirac}, H_{\rm Dirac}), \text{ with } H_{\rm Dirac} = \begin{pmatrix} 0 & 2D_z \\ 2D_{\bar z} & 0 \end{pmatrix}.$$

Since honeycomb lattices are unions of two triangular lattices, we may distinguish between atoms of type A and B. Considering then only the tunnelling interaction of atoms of different types between the layers gives rise to an off-diagonal tunnelling matrix

$$\tau(\alpha, z) = \begin{pmatrix} 0 & \alpha\overline{U(-z)} \\ \alpha U(z) & 0 \end{pmatrix}.$$

The tunnelling potential is then described by

$$H_{\rm tun}(\alpha) = \begin{pmatrix} 0 & \tau(\alpha, z) \\ \tau(\alpha, z)^* & 0 \end{pmatrix}.$$

Conjugating the sum of the two Hamiltonians by unitary operators yields, for $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$,

$$H(\alpha) = \operatorname{diag}(1, \sigma_1, 1)(H_{\rm kin} + H_{\rm tun}(\alpha)) \operatorname{diag}(1, \sigma_1, 1),$$

which is the operator introduced in [TKV19] and studied in this article.

2.1. **Symmetries of $H(\alpha)$.** The potential (1.2) satisfies the following properties:

$$\begin{gathered} \mathbf{a} = \tfrac{4}{3}\pi i \omega^\ell, \ \ell = 1, 2 \implies U(z + \mathbf{a}) = \bar\omega U(z), \text{ and} \\ U(\omega z) = \omega U(z). \end{gathered} \tag{2.1}$$

The first property in (2.1) follows from the fact that (with $k, \ell \in \mathbb{Z}_3$)

$$\tfrac{1}{2}(\mathbf{a}\bar\omega^k - \bar{\mathbf{a}}\omega^k) = \tfrac{2}{3}\pi i(\omega^{k-\ell} + \bar\omega^{k-\ell}) = \begin{cases} \tfrac{4}{3}\pi i \equiv -\tfrac{2}{3}\pi i \mod 2\pi i, & k - \ell = 0; \\ -\tfrac{2}{3}\pi i, & k - \ell \neq 0. \end{cases}$$

From this first property in (2.1) we see that

$$U(z + \gamma) = U(z), \quad \gamma \in \Gamma := 4\pi \left(i\omega\mathbb{Z} \oplus i\omega^2\mathbb{Z} \right). \tag{2.2}$$

The dual lattice consisting of $\mathbf{k}$ satisfying $\frac{1}{2}(\gamma\bar{\mathbf{k}}+\bar{\gamma}\mathbf{k})\in 2\pi\mathbb{Z}$ for $\gamma\in\Gamma$, is given by $\Gamma^*=\frac{1}{\sqrt{3}}(\omega\mathbb{Z}\oplus\omega^2\mathbb{Z})$.

The second identity in (2.1) shows that with $L_{\mathbf{a}}\mathbf{v}(z):=\mathbf{v}(z+\mathbf{a})$,

$$D(\alpha)L_{\mathbf{a}}=L_{\mathbf{a}}\begin{pmatrix}2D_{\bar z} & \omega\alpha U\\ \bar\omega\alpha U(-\bullet) & 2D_{\bar z}\end{pmatrix}=\begin{pmatrix}\omega & 0\\ 0 & 1\end{pmatrix}L_{\mathbf{a}}D(\alpha)\begin{pmatrix}\bar\omega & 0\\ 0 & 1\end{pmatrix},\quad \mathbf{a}=\tfrac{4}{3}\pi i\omega^\ell,\quad \ell=1,2.$$

Hence,

$$\mathscr{L}_{\mathbf{a}}D(\alpha)=D(\alpha)\mathscr{L}_{\mathbf{a}},\quad \mathscr{L}_{\mathbf{a}}:=\begin{pmatrix}\omega & 0\\ 0 & 1\end{pmatrix}L_{\mathbf{a}},\quad \mathbf{a}=\tfrac{4}{3}\pi i\omega^\ell,\quad \ell=1,2. \tag{2.3}$$

Putting

$$\Gamma_3:=\Gamma/3=\tfrac{4}{3}\pi(i\omega\mathbb{Z}\oplus i\omega^2\mathbb{Z}),\quad \Gamma_3/\Gamma\simeq\mathbb{Z}_3^2, \tag{2.4}$$

and

$$\mathscr{L}_{\mathbf{a}}:=\begin{pmatrix}\omega^{a_1+a_2} & 0\\ 0 & 1\end{pmatrix}L_{\mathbf{a}},\quad \mathbf{a}=\tfrac{4}{3}\pi i(\omega a_1+\omega^2 a_2),$$

we obtain a unitary action of Γ_3 on $L^2(\mathbb{C})$ or on $L^2(\mathbb{C}/\Gamma)$, $\Gamma_3\ni\mathbf{a}\mapsto\mathscr{L}_{\mathbf{a}}$.

We extend the action of $\mathscr{L}_{\mathbf{a}}$ to $L^2(\mathbb{C};\mathbb{C}^4)$ or $L^2(\mathbb{C}/\Gamma;\mathbb{C}^4)$ block-diagonally and we have $\mathscr{L}_{\mathbf{a}}H(\alpha)=H(\alpha)\mathscr{L}_{\mathbf{a}}$.

The second identity in (2.1) shows that $[D(\alpha)\mathbf{u}(\omega\bullet)](z)=\bar\omega[D(\alpha)\mathbf{u}](\omega z)$. Hence,

$$\mathscr{C}H(\alpha)=H(\alpha)\mathscr{C},\qquad \mathscr{C}\mathbf{u}(z):=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&\bar\omega&0\\0&0&0&\bar\omega\end{pmatrix}\mathbf{u}(\omega z),\quad \mathbf{u}\in L^2(\mathbb{C};\mathbb{C}^4).$$

Since $\mathscr{C}\mathscr{L}_{\mathbf{a}}=\mathscr{L}_{\bar\omega\mathbf{a}}\mathscr{C}$, we combine the two actions into a unitary group action that commutes with $D(\alpha)$:

$$\begin{gathered}G:=\Gamma_3\rtimes\mathbb{Z}_3,\quad \mathbb{Z}_3\ni k:\mathbf{a}\to\bar\omega^k\mathbf{a},\quad (\mathbf{a},k)\cdot(\mathbf{a}',\ell)=(\mathbf{a}+\bar\omega^k\mathbf{a}',k+\ell),\\ (\mathbf{a},\ell)\cdot\mathbf{u}=\mathscr{L}_{\mathbf{a}}\mathscr{C}^\ell\mathbf{u}.\end{gathered} \tag{2.5}$$

By taking a quotient by Γ we obtain a finite group acting unitarily on $L^2(\mathbb{C}/\Gamma)$ and commuting with $H(\alpha)$:

$$G_3:=G/\Gamma=\Gamma_3/\Gamma\rtimes\mathbb{Z}_3\simeq\mathbb{Z}_3^2\rtimes\mathbb{Z}_3. \tag{2.6}$$

By restriction to the first two components, G and G_3 act on $L^2(\mathbb{C};\mathbb{C})$ and $L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)$ as well and we use the same notation for those actions.

Remark. The group G_3 is naturally identified with the finite Heisenberg group He_3:

$$\mathrm{He}_3 := \left\{ \begin{pmatrix} 1 & x & t \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix}, \ x, y, t \in \mathbb{Z}_3 \right\},$$

$$\begin{pmatrix} 1 & x & t \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & x' & t' \\ 0 & 1 & y' \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & x+x' & t+t'+xy' \\ 0 & 1 & y+y' \\ 0 & 0 & 1 \end{pmatrix}.$$

The identification of G_3 and He_3 follows: with $\Gamma_3/\Gamma \ni \mathbf{a} \mapsto F(\mathbf{a}) := (a_1, a_2) \in \mathbb{Z}_3^2$, $\mathbf{a} = \frac{4}{3}\pi i(\omega a_1 + \omega^2 a_2)$, we have $\mathrm{He}_3 \ni (x, y, t) \longmapsto (F^{-1}(t, y-t), x) \in G_3$. □

We record two more actions involving $H(\alpha)$:

$$H(\alpha) = -\mathscr{W} H(\alpha) \mathscr{W}^*, \quad \mathscr{W} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathscr{W}\mathscr{C} = \mathscr{C}\mathscr{W}, \quad \mathscr{L}_{\mathbf{a}}\mathscr{W} = \mathscr{W}\mathscr{L}_{\mathbf{a}}, \tag{2.7}$$

and

$$\mathscr{Q} H(\alpha) \mathscr{Q}^* = -H(-\alpha), \quad \mathscr{Q} := \operatorname{diag}(i, -i, -i, i), \quad \mathscr{Q}\mathscr{C} = \mathscr{C}\mathscr{Q}, \quad \mathscr{Q}\mathscr{L}_{\mathbf{a}} = \mathscr{L}_{\mathbf{a}}\mathscr{Q}.$$

We summarize these simple findings in

Proposition 2.1. *The operator $H(\alpha) : L^2(\mathbb{C}; \mathbb{C}^4) \to L^2(\mathbb{C}; \mathbb{C}^4)$ is an unbounded self-adjoint operator with the domain given by $H^1(\mathbb{C}; \mathbb{C}^4)$. The operator $H(\alpha)$ commutes with the unitary action of the group G given by (2.5) and*

$$\operatorname{Spec}_{L^2(\mathbb{C})} H(\alpha) = -\operatorname{Spec}_{L^2(\mathbb{C})} H(\alpha) = \operatorname{Spec}_{L^2(\mathbb{C})} H(-\alpha).$$

The same conclusions are valid when $L^2(\mathbb{C})$ is replaced by $L^2(\mathbb{C}/\Gamma)$ and G by G_3 given by (2.6). In addition, the spectrum is then discrete.

2.2. **Representation theory and protected states at 0.** Irreducible unitary representations of $\mathbb{Z}_3^2$ are one dimensional and are given by

$$\begin{gathered} \pi_{\mathbf{k}} : \mathbb{Z}_3^2 \to \mathsf{U}(1), \quad \pi_{\mathbf{k}}(\mathbf{a}) = e^{\frac{i}{2}(\mathbf{a}\bar{\mathbf{k}} + \bar{\mathbf{a}}\mathbf{k})}, \\ \mathbf{a} = \tfrac{4}{3}\pi(a_1 i\omega + a_2 i\omega^2), \quad a_j \in \mathbb{Z}_3, \quad \mathbf{k} = \tfrac{1}{\sqrt{3}}(\omega^2 k_1 - \omega k_2), \ k_j \in \mathbb{Z}_3, \\ \tfrac{1}{2}(\mathbf{a}\bar{\mathbf{k}} + \bar{\mathbf{a}}\mathbf{k}) = \langle \mathbf{a}, \mathbf{k} \rangle = \tfrac{2\pi}{3}(k_1 a_1 + k_2 a_2). \end{gathered} \tag{2.8}$$

Irreducible representations of G_3 are one dimensional for $\mathbf{k} \in \Delta$ (given by $\Delta(\mathbb{Z}_3) := \{(k, k), k \in \mathbb{Z}_3\}$ – we note that $\langle \mathbf{k}, \omega\mathbf{a} \rangle = \langle \mathbf{k}, \mathbf{a} \rangle$, $\mathbf{a} \in \Gamma_3/\Gamma$, if and only if $\mathbf{k} \in \Delta$),

$$\rho_{k,p}((\mathbf{a}, \ell)) = \bar{\omega}^{\ell p} \pi_{(k,k)}(\mathbf{a}),$$

or three dimensional, for $\mathbf{k} \notin \Delta$:

$$\rho_{\mathbf{k}}((\mathbf{a}, \ell)) = \begin{pmatrix} \omega^{\langle \mathbf{k}, \mathbf{a} \rangle} & 0 & 0 \\ 0 & \omega^{\langle \mathbf{k}, \omega\mathbf{a} \rangle} & 0 \\ 0 & 0 & \omega^{\langle \mathbf{k}, \omega^2\mathbf{a} \rangle} \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}^{\ell} \in \mathsf{U}(3).$$

The representations are equivalent for $\mathbf{k}$ in the same orbit of the transpose of $\mathbf{a} \mapsto \omega \mathbf{a}$, and hence there are only two.

From this we see the well known fact that there are 11 irreducible representations: 9 one dimensional and 2 three dimensional. We can decompose $L^2(\mathbb{C}/\Gamma; \mathbb{C}^4)$ into 11 orthogonal subspaces (since the groups are finite we do not have the usual Floquet theory difficulties!):

$$L^2(\mathbb{C}/\Gamma; \mathbb{C}^4) = \bigoplus_{k,p \in \mathbb{Z}_3} L^2_{\rho_{k,p}}(\mathbb{C}/\Gamma; \mathbb{C}^4) \oplus L^2_{\rho_{(1,0)}}(\mathbb{C}/\Gamma; \mathbb{C}^4) \oplus L^2_{\rho_{(2,0)}}(\mathbb{C}/\Gamma; \mathbb{C}^4).$$

In view of Proposition 2.1 we have

$$H_{k,p}(\alpha) := H(\alpha) : (L^2_{\rho_{k,p}} \cap H^1)(\mathbb{C}/\Gamma; \mathbb{C}^4) \to L^2_{\rho_{k,p}}(\mathbb{C}/\Gamma; \mathbb{C}^4),$$

with similarly defined $H_{(1,0)}$ and $H_{(0,1)}$.

We now consider the case of $\alpha = 0$ and analyse $\ker_{L^2(\mathbb{C}/\Gamma)} H(0)$ decomposed into the corresponding representations:

$$\ker_{L^2(\mathbb{C}/\Gamma)} H(0) = \{\mathbf{u} = \mathbf{e}_j, \ j = 1, \ldots, 4\},$$

where the $\mathbf{e}_j$ form the standard basis elements of $\mathbb{C}^4$. The action of $G_3 = \mathbb{Z}_3^2 \rtimes \mathbb{Z}_3$ is diagonal and, with $\mathbf{a} = \frac{4}{3}\pi(a_1 i\omega + a_2 i\omega^2)$,

$$\begin{gathered} \mathscr{L}_{\mathbf{a}} \mathbf{e}_1 = \omega^{a_1+a_2} \mathbf{e}_1, \quad \mathscr{L}_{\mathbf{a}} \mathbf{e}_2 = \mathbf{e}_2, \quad \mathscr{L}_{\mathbf{a}} \mathbf{e}_3 = \omega^{a_1+a_2} \mathbf{e}_3, \quad \mathscr{L}_{\mathbf{a}} \mathbf{e}_4 = \mathbf{e}_4, \\ \mathscr{C} \mathbf{e}_1 = \mathbf{e}_1, \quad \mathscr{C} \mathbf{e}_2 = \mathbf{e}_2, \quad \mathscr{C} \mathbf{e}_3 = \bar{\omega} \mathbf{e}_3, \quad \mathscr{C} \mathbf{e}_4 = \bar{\omega} \mathbf{e}_4. \end{gathered}$$

These observations imply that, with $L^2_{\rho_{k,p}} := L^2_{\rho_{k,p}}(\mathbb{C}/\Gamma; \mathbb{C}^4)$,

$$\mathbf{e}_1 \in L^2_{\rho_{1,0}}, \quad \mathbf{e}_2 \in L^2_{\rho_{0,0}}, \quad \mathbf{e}_3 \in L^2_{\rho_{1,1}}, \quad \mathbf{e}_4 \in L^2_{\rho_{0,1}}.$$

Hence for $\alpha = 0$, each of $H_{0,0}(0)$, $H_{1,0}(0)$, $H_{0,1}(0)$ and $H_{1,1}(0)$ has a simple eigenvalue at 0. Since $\mathscr{W}$ (see (2.7)) commutes with the action of G_3, the spectra of $H_{k,\ell}(\alpha)$ are symmetric with respect to 0, it follows that $H_{k,\ell}(\alpha)$, k, ℓ as above, each have an eigenvalue at 0.

Since $\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^4)} H(\alpha) = \ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha) \oplus \{0_{\mathbb{C}^2}\} + \{0_{\mathbb{C}^2}\} \oplus \ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha)^*$, we obtained the following result about a symmetry protected eigenstate at 0:

Proposition 2.2. *For all $\alpha \in \mathbb{C}$,*

$$\ker_{L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha) \neq \{0\}.$$

In the notation of (1.6), $\ker_{L^2_{\rho_{0,0}}(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha) = \mathscr{E} \ker_{L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha) \neq \{0\}$.

2.3. **Floquet theory.** Since the statement (1.4) is interpreted as having a "flat Floquet band" at zero energy, we conclude this section with a brief account of Floquet theory.

In principle, we could use the unitarity dual of G defined in (2.5) (and described similarly to the unitary dual of G_3 in §2.2) and decompose $L^2(\mathbb{C})$ into irreducible representations under the action of G. However, let us take the standard Floquet theory approach based on invariance under Γ (see (2.2))

$$\Gamma \ni \mathbf{a} : \psi \longmapsto \mathscr{L}_{\mathbf{a}} \psi(z) = \psi(z+\mathbf{a}), \quad \psi \in L^2(\mathbb{C};\mathbb{C}^2), \quad D(\alpha)\mathscr{L}_{\mathbf{a}} = \mathscr{L}_{\mathbf{a}} D(\alpha).$$

(This definition agrees with (2.3) when $\mathbf{a} \in \Gamma$.)

We start by recording basic properties of the operator $D(\alpha)$. We first observe that

$$\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)} D(0) = \Gamma^*, \quad D(0) e_{\mathbf{k}} \mathbf{e}_j = \mathbf{k} e_{\mathbf{k}} \mathbf{e}_j, \quad e_{\mathbf{k}}(z) := e^{\frac{i}{2}(\bar{\mathbf{k}} z + \mathbf{k}\bar{z})}, \quad \mathbf{k} \in \Gamma^*, \quad j = 1, 2, \tag{2.9}$$

where the exponentials $e_{\mathbf{k}} / \operatorname{vol}(\mathbb{C}/\Gamma)^{\frac{1}{2}}$ form an orthonormal basis of $L^2(\mathbb{C}/\Gamma)$ and $\mathbf{e}_j$ are the standard basis of $\mathbb{C}^2$.

We then have the following simple

Proposition 2.3. *The family $\mathbb{C} \ni \alpha \mapsto D(\alpha) : H^1(\mathbb{C}/\Gamma;\mathbb{C}^2) \to L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)$ is a holomorphic family of elliptic Fredholm operators of index 0, and for all α, the spectrum of $D(\alpha)$ is Γ^*-periodic:*

$$\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) + \mathbf{k}, \quad \mathbf{k} \in \Gamma^*. \tag{2.10}$$

Proof. Since $D_{\bar{z}}$ is an elliptic operator in dimension 2, existence of parametrices (see for instance [DyZw19, Proposition E.32]) immediately shows the Fredholm property (see for instance [DyZw19, §C.2] for that and other basic properties of Fredholm operators). In view of (2.9), $D(0) - \mathbf{k}$ is invertible for $\mathbf{k} \notin \Gamma^*$ and hence $D(0) : H^1(\mathbb{C}/\Gamma) \to L^2(\mathbb{C}/\Gamma)$ is an operator of index 0. The same is true for the Fredholm family $D(\alpha)$. To see (2.10), note that if $(D(\alpha) - \lambda)\mathbf{u} = 0$ then $(D(\alpha) - (\lambda + \mathbf{k}))(e_{\mathbf{k}}\mathbf{u}) = 0$, $\mathbf{k} \in \Gamma^*$. □

For $\mathbf{k} \in \mathbb{C}/\Gamma^*$ (or simply $\mathbf{k} \in \mathbb{C}$) we defined the Floquet boundary condition as

$$\psi(z+\mathbf{a}) = e^{-\frac{i}{2}(\mathbf{a}\bar{\mathbf{k}} + \bar{\mathbf{a}}\mathbf{k})} \psi(z), \quad \psi \in L^2_{\mathrm{loc}}(\mathbb{C};\mathbb{C}^2), \quad \mathbf{a} \in \Gamma.$$

This means that

$$\mathbf{v}(z) := e^{\frac{i}{2}(z\bar{\mathbf{k}} + \bar{z}\mathbf{k})} \psi(z)$$

satisfies

$$\mathbf{v}(z+\mathbf{a}) = \mathbf{v}(z), \quad \mathbf{a} \in \Gamma, \quad e^{\frac{i}{2}(z\bar{\mathbf{k}} + \bar{z}\mathbf{k})} D(\alpha)\psi(z) = (D(\alpha) - \mathbf{k})\mathbf{v}(z).$$

It follows that

$$e^{\frac{i}{2}(z\bar{\mathbf{k}} + \bar{z}\mathbf{k})} H(\alpha) e^{\frac{i}{2}(z\bar{\mathbf{k}} + \bar{z}\mathbf{k})} = H_{\mathbf{k}}(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* - \bar{\mathbf{k}} \\ D(\alpha) - \mathbf{k} & 0 \end{pmatrix}, \tag{2.11}$$

where $H_{\mathbf{k}}(\alpha)$ is the operator in (1.4).

We now proceed with standard Floquet theory and introduce the unitary transformation

$$\mathscr{U} : L^2(\mathbb{C};\mathbb{C}^4) \to L^2(\mathbb{C}/\Gamma^*; L^2(\mathbb{C}/\Gamma)), \quad \mathscr{U}\mathbf{u}(\mathbf{k}, z) := \sum_{\mathbf{a}\in\Gamma} u(z+\mathbf{a}) e^{\frac{i}{2}((z+\mathbf{a})\bar{\mathbf{k}}+(\bar{z}+\bar{\mathbf{a}})\mathbf{k})}.$$

We then have

$$\mathscr{U} H \mathscr{U}^* \mathbf{v}(z,\mathbf{k}) = H_{\mathbf{k}} \mathbf{v}(z,\mathbf{k}), \quad \mathbf{v}(\bullet,\mathbf{k}) \in C^\infty(\mathbb{C}/\Gamma;\mathbb{C}^4),$$

that is, for a fixed $\mathbf{k} \in \mathbb{C}/\Gamma^*$, $\mathscr{U} H \mathscr{U}^*$ acts on *periodic functions with respect to* Γ as the operator in (2.11). For each $\mathbf{k}$, the operator $H_{\mathbf{k}}(\alpha)$ is an elliptic differential system (see Proposition 2.3 above) and hence it has a discrete spectrum that then describes the spectrum of $H(\alpha)$ on $L^2(\mathbb{C})$:

$$\begin{gathered} \operatorname{Spec}_{L^2(\mathbb{C})}(H(\alpha)) = \bigcup_{\mathbf{k}\in\mathbb{C}/\Gamma^*} \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_{\mathbf{k}}(\alpha)), \\ \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_{\mathbf{k}}(\alpha)) = \{\pm E_j(\mathbf{k},\alpha)\}_{j=0}^\infty, \quad E_{j+1}(\mathbf{k},\alpha) \geq E_j(\mathbf{k},\alpha) \geq 0. \end{gathered} \tag{2.12}$$

To see the last statement we recall that

$$(\lambda - \mathscr{A})^{-1} = \begin{pmatrix} (\lambda^2 - A^*A)^{-1} & 0 \\ 0 & (\lambda^2 - AA^*)^{-1} \end{pmatrix} \begin{pmatrix} \lambda & A^* \\ A & \lambda \end{pmatrix}, \quad \mathscr{A} := \begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}.$$

Hence, the non-zero eigenvalues of $H_{\mathbf{k}}$ are given by $\pm$ the non-zero singular values of $D(\alpha)+\mathbf{k}$ (that is, the eigenvalues of $[(D(\alpha)+\mathbf{k})^*(D(\alpha)+\mathbf{k})]^{\frac{1}{2}}$), included according to their multiplicities). We need to check that the eigenvalue 0 of $(D(\alpha)+\mathbf{k})^*(D(\alpha)+\mathbf{k})$ has the same multiplicity as the zero eigenvalue of $(D(\alpha)+\mathbf{k})(D(\alpha)+\mathbf{k})^*$, so that eigenvalues $E_j(\mathbf{k},\alpha) = 0$ are included exactly twice (for $\pm$).

For that we use Proposition 2.3, which also shows that $D(\alpha)+\mathbf{k}$ is a Fredholm operator of order zero, and hence

$$\dim\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)}(D(\alpha)+\mathbf{k}) = \dim\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)}(D(\alpha)^* + \bar{\mathbf{k}}).$$

In (2.12) we abuse notation by counting ± 0 twice in the spectrum of $H_{\mathbf{k}}(\alpha)$.

From this discussion we can re-interpret (1.4) as the existence of a flat band:

Proposition 2.4. *In the notation of* (1.4) *and* (2.12)

$$0 \in \bigcap_{\mathbf{k}\in\mathbb{C}} \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma,\mathbb{C}^4)} H_{\mathbf{k}}(\alpha) \iff E_0(\mathbf{k},\alpha) = 0 \textit{ for all } \mathbf{k} \in \mathbb{C}/\Gamma^*. \tag{2.13}$$

3. Resonant and magic angles

We now want to obtain a computable condition on α guaranteeing (1.4), that is, the flatness of a band (2.13). In view of (2.11) and (2.12), (1.4) is equivalent to $\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \mathbb{C}$.

3.1. **Spectrum of $D(\alpha)$.** To investigate the spectrum of $D(\alpha)$ we use the operator $T_{\mathbf{k}}$ defined in (1.9). We note that for $\mathbf{k} \notin \Gamma^*$, (2.9) shows that

$$D(\alpha) - \mathbf{k} = (D(0) - \mathbf{k})(I + \alpha T_{\mathbf{k}}), \quad D(0) = 2D_{\bar{z}}. \tag{3.1}$$

The operator $T_{\mathbf{k}} : L^2(\mathbb{C}/\Gamma; \mathbb{C}^2) \to L^2(\mathbb{C}/\Gamma; \mathbb{C}^2)$ is compact and hence its spectrum can only accumulate at 0. This means that

$$\Gamma^* \not\ni \mathbf{k} \in \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) \iff \alpha \in \mathcal{A}_{\mathbf{k}}, \quad \mathcal{A}_{\mathbf{k}} := 1/(\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(T_{\mathbf{k}}) \setminus \{0\}), \tag{3.2}$$

where $\mathcal{A}_{\mathbf{k}}$ is a discrete subset of $\mathbb{C}$.

We now have a proposition proving the first part of Theorem 2. It also defines the family of functions appearing in Theorem 1.

Proposition 3.1. *For $\mathbf{k} \notin \Gamma^*$, the discrete set $\mathcal{A} = \mathcal{A}_{\mathbf{k}}$ is* independent *of $\mathbf{k}$ and*

$$\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(D(\alpha)) = \begin{cases} \Gamma^*, & \alpha \notin \mathcal{A}; \\ \mathbb{C}, & \alpha \in \mathcal{A}. \end{cases} \tag{3.3}$$

Moreover, for all $\alpha \notin \mathcal{A}$,

$$\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha) = \mathbb{C}\mathbf{u}(\alpha) \oplus \mathbb{C}\mathscr{E}\mathbf{u}(\alpha), \quad \mathbf{u}(\alpha) \in L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma; \mathbb{C}^2), \quad \mathbf{u}(0) = \mathbf{e}_1, \tag{3.4}$$

where $\mathscr{E}$ is defined in (1.6) and $\mathbf{e}_1 = (1,0)^t$. For $\alpha \in \mathbb{R}$, $\mathbf{u}$ extends to a real analytic family, $\mathbb{R} \ni \alpha \mapsto \mathbf{u}(\alpha) \in \ker_{L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha)$.

Proof. Suppose $\alpha \in \mathbb{C} \setminus \mathcal{A}_{\mathbf{k}}$, $\mathbf{k} \notin \Gamma^*$. Then $(D(\alpha) - \mathbf{k})^{-1} : L^2(\mathbb{C}/\Gamma) \to H^1(\mathbb{C}/\Gamma) \hookrightarrow L^2(\mathbb{C}/\Gamma)$ is a compact operator and hence $D(\alpha)$ has discrete spectrum. By Proposition 2.2, $0 \in \operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(D(\alpha))$ for all $\alpha \in \mathbb{C}$, and thus together with the periodicity condition (2.10) this implies $\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}(D(\alpha)) \supset \Gamma^*$. Recall now that $D(\alpha)$ depends on α holomorphically and 0 is isolated in the spectrum for $\alpha \notin \mathcal{A}_{\mathbf{k}}$. Thus, $\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha)$ depends holomorphically on $\alpha \notin \mathcal{A}_{\mathbf{k}}$ [Ka80, VII. Theorem 1.7] and by Proposition 2.2 $\dim(\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha)) \geq 2$ for all $\alpha \in \mathbb{C}$, we find

$$\dim(\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha)) = \dim(\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(0)) = 2 \text{ for all } \alpha \notin \mathcal{A}_{\mathbf{k}}.$$

The discreteness of the spectrum implies that the spectrum depends continuously on α [Ka80, II. 6] for $\alpha \notin \mathcal{A}_{\mathbf{k}}$. Since $\dim(\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha)) = 2$ for all $\alpha \notin \mathcal{A}_{\mathbf{k}}$ and by periodicity (2.10), this implies that $\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma,\mathbb{C}^2)}(D(\alpha)) = \Gamma^*$.

Using (3.2) and that $\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma,\mathbb{C}^2)}(D(\alpha)) = \Gamma^*$ for all $\alpha \notin \mathcal{A}_{\mathbf{k}}$, it follows that

$$\exists\, \mathbf{k} \notin \Gamma^* \ \text{ such that } \ \alpha \notin \mathcal{A}_{\mathbf{k}} \implies \forall\, \mathbf{p} \notin \Gamma^* \ \text{ we have } \ \alpha \notin \mathcal{A}_{\mathbf{p}}.$$

This shows independence of $\mathcal{A}_{\mathbf{k}} =: \mathcal{A}$ of $\mathbf{k}$.

Since

$$\mathbb{C} \ni \alpha \mapsto \widetilde{H}(\alpha) := \begin{pmatrix} 0 & D(\bar{\alpha})^* \\ D(\alpha) & 0 \end{pmatrix}, \quad \widetilde{H}(\alpha) = H(\alpha), \quad \alpha \in \mathbb{R},$$

is a holomorphic operator family with compact resolvents, self-adjoint for $\alpha \in \mathbb{R}$, Rellich's theorem [Ka80, VII. Theorem 3.9] implies that all eigenvalues and eigenfunctions of $H(\alpha) = \widetilde{H}(\alpha)$ can be chosen to depend real-analytically on $\alpha \in \mathbb{R}$. If we let $\varphi(\alpha) := (\mathbf{u}(\alpha), 0, 0)^t \in L^2_{\rho_{1,0}}$, $\alpha \in \mathbb{R} \setminus \mathcal{A}$, then $\varphi(0) = \mathbf{e}_1 \in \mathbb{C}^4$ and by the discussion above $\varphi(\alpha)$ extends to a real analytic family for all $\alpha \in \mathbb{R}$. $\square$

The next proposition provides the symmetries of the set $\mathcal{A}$.

Proposition 3.2. *Suppose that in addition to (2.1) we have $U(z) = \overline{U(\bar z)}$. Then,* $\operatorname{Spec} D(\alpha) = \operatorname{Spec} D(-\alpha) = \operatorname{Spec} D(\bar\alpha)$ *and hence*

$$\mathcal{A} = -\mathcal{A} = \overline{\mathcal{A}}.$$

In these statements Spec *can be either the spectrum on* $L^2(\mathbb{C})$, $\operatorname{Spec}_{L^2(\mathbb{C})}$, *or on* $L^2(\mathbb{C}/\Gamma)$, $\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)}$.

Proof. To see the symmetries of the spectrum, we note that since $Q\mathbf{v}(z) = \overline{\mathbf{v}(-z)}$, the anti-linear involution satisfies

$$D(\alpha)Q\mathbf{v} = -QD(-\alpha)^*\mathbf{v},$$

which in turn implies $\operatorname{Spec} D(\alpha) = -\overline{\operatorname{Spec}} D(-\alpha)^* = -\operatorname{Spec} D(-\alpha)$. But then (3.3) shows that $\operatorname{Spec} D(\alpha) = \operatorname{Spec} D(-\alpha)$.

Next we notice that $\overline{U(\bar z)} = U(z)$. If we define the unitary map $F\mathbf{v}(z) := \overline{\mathbf{v}(\bar z)}$, then we find using $(D_{\bar z}F\mathbf{v})(z) = (D_z\overline{\mathbf{v}})(\bar z) = -(\overline{D_{\bar z}\mathbf{v}})(\bar z) = -(FD_{\bar z}\mathbf{v})(z)$ the relation

$$D(\alpha)(F\mathbf{v}) = -F(D(-\bar\alpha)\mathbf{v}),$$

which implies that $\operatorname{Spec}(D(\alpha)) = -\operatorname{Spec}(D(-\bar\alpha)) = \operatorname{Spec}(D(\bar\alpha))$. $\square$

The description of the kernel of $D(\alpha)$ gives us an expression for the inverse of $D(\alpha) - \mathbf{k}$, $\mathbf{k} \notin \Gamma^*$ and $\alpha \notin \mathcal{A}$. We start with the following simple

Proposition 3.3. *Suppose that $\mathbf{u}(\alpha)$ is given in (3.4) and define a two-by-two matrix*

$$\mathbf{V}(\alpha) := [\mathbf{u}(\alpha), \mathscr{E}\mathbf{u}(\alpha)], \quad v(\alpha) := \det \mathbf{V}(\alpha).$$

Then $v(\alpha) \neq 0$ and $\mathbf{k} \notin \Gamma^*$ imply that, with the cofactor matrix denoted by adj,

$$(D(\alpha) - \mathbf{k})^{-1} = \frac{1}{v(\alpha)} \operatorname{adj}(\mathbf{V}(\alpha))(2D_{\bar z} - \mathbf{k})^{-1}(\mathbf{V}(\alpha)). \tag{3.5}$$

For a fixed $\mathbf{k} \notin \Gamma^*$, $\alpha \mapsto (D(\alpha) - \mathbf{k})^{-1}$ is a meromorphic family of compact operators with poles of finite rank at $\alpha \in \mathcal{A}$.

Proof. If $v(\alpha) \neq 0$, then $\mathbf{V}(\alpha)^{-1} = \operatorname{adj}\mathbf{V}(\alpha)/v(\alpha)$ and (3.5) follows from a simple calculation ($\mathbf{V}(\alpha)$ provides a matrix-valued integrating factor). In view of (3.1),

$$(D(\alpha) - \mathbf{k})^{-1} = (I + \alpha T_{\mathbf{k}})^{-1}(D(0) - \mathbf{k})^{-1},$$

where, using analytic Fredholm theory (see for instance [DyZw19, Theorem C.8]), $\alpha \mapsto (I + \alpha T_{\mathbf{k}})^{-1}$ is a meromorphic family of operators with poles of finite rank. $\square$

The proposition shows that $\alpha \in \mathcal{A}$ implies that $v(\alpha) = 0$. To obtain the opposite implication (which then gives Theorem 1) we will use the theta function argument from [TKV19].

3.2. **A theta function argument.** We first review basic definitions and properties of θ functions – see [Mu83]. We have

$$\begin{gathered}\theta_{a,b}(z|\tau) := \sum_{n\in\mathbb{Z}} \exp(\pi i(a+n)^2\tau + 2\pi i(n+a)(z+b)), \quad \operatorname{Im}\tau > 0, \\ \theta_{a,b}(z+1|\tau) = e^{2\pi i a}\theta_{a,b}(z|\tau), \quad \theta_{a,b}(z+\tau|\tau) = e^{-2\pi i(z+b)-\pi i\tau}\theta_{a,b}(z|\tau), \\ \theta_{a+1,b}(z|\tau) = \theta_{a,b}(z|\tau), \quad \theta_{a,b+1}(z|\tau) = e^{2\pi i a}\theta_{a,b}(z|\tau).\end{gathered} \tag{3.6}$$

The (simple) zeros of the (entire) function $z \mapsto \theta_{a,b}(z|\tau)$ are given by

$$z_{n,m} = (n - \tfrac{1}{2} - a)\tau + \tfrac{1}{2} - b - m. \tag{3.7}$$

If

$$g(z) := \frac{\theta_{a',b'}(z/\tau'|\tau)}{\theta_{a,b}(z/\tau'|\tau)}, \tag{3.8}$$

then (3.6) shows that

$$g(z+\tau') = e^{2\pi i(a'-a)}g(z), \quad g(z+\tau\tau') = e^{-2\pi i(b'-b)}g(z), \tag{3.9}$$

and from (3.7) we know the zeros and poles of g.

With this in place we can prove

Proposition 3.4. *In the notation of Propositions 3.1 and 3.3 we have*

$$v(\alpha) = 0, \quad \alpha \in \mathbb{R} \implies \alpha \in \mathcal{A}.$$

Proof. If $\mathbf{u}(\alpha) = (\psi_1, \psi_2)$ then

$$v(\alpha) = \psi_1(z)\psi_1(-z) + \psi_2(z)\psi_2(-z).$$

As remarked after (1.5), $v(\alpha)$ is independent of z.

The observation made in [TKV19] is that ψ_2 vanishes at special *stacking* points. These are fixed points of the action $z \mapsto \omega z$ on $\mathbb{C}/\Gamma_3$ (see (2.4)):

$$\psi_2(\alpha, \pm z_S) = 0, \quad z_S := \tfrac{1}{3}(\mathbf{a}_2 - \mathbf{a}_1) = \tfrac{4\sqrt{3}}{9}\pi, \quad \mathbf{a}_j = \tfrac{4}{3}\pi i\omega^j. \tag{3.10}$$

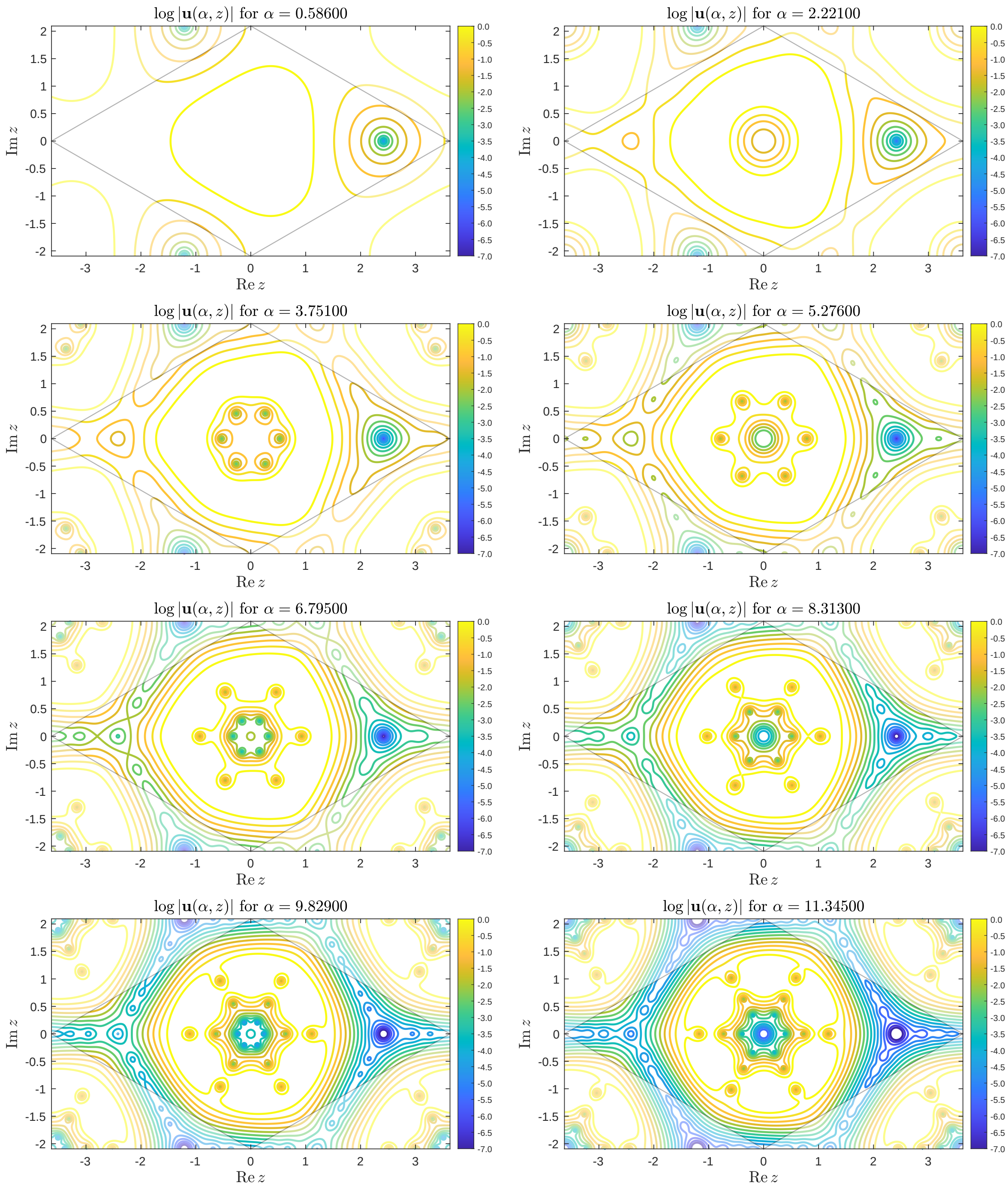

FIGURE 5. Plots of $z \mapsto \log|\mathbf{u}(\alpha, z)|$ (in the notation of Proposition 3.1) for α *close* to magic values (due to pseudospectral effects it is difficult to compute the exact eigenfunction at a magic angle) showing that the value of $\mathbf{u}$ at $z_S = \frac{4\sqrt{3}}{9}\pi$ is close to 0.

To see this, note that (with the action of $\mathscr{C}$ identified with the action on $(\mathbf{u}, 0_{\mathbb{C}^2})^t \in L^2(\mathbb{C}/\Gamma; \mathbb{C}^4)$)

$$\begin{aligned}\mathbf{u}(\alpha, \pm z_S) &= \mathscr{C}\mathbf{u}(\alpha, \pm z_S) = \mathbf{u}(\alpha, \pm\omega z_S) = \mathbf{u}(\alpha, \pm z_S \mp \mathbf{a}_2) \\ &= \begin{pmatrix} \omega^{\pm 1} & 0 \\ 0 & 1 \end{pmatrix} \mathscr{L}_{\mp\mathbf{a}_2}\mathbf{u}(\alpha, \pm z_S) = \begin{pmatrix} 1 & 0 \\ 0 & \omega^{\mp 1} \end{pmatrix} \mathbf{u}(\alpha, \pm z_S).\end{aligned}$$

Hence $\psi_2(\pm z_S) = \omega^{\mp 1}\psi_2(\pm z_S)$, which proves (3.10).

We conclude that if $v(\alpha) = 0$ then $\psi_1(z_S)\psi_1(-z_S) = 0$, and hence $\mathbf{u}(\alpha, z_S) = 0$ or $\mathbf{u}(\alpha, -z_S) = 0$. Assume the former holds (otherwise we replace $\mathbf{u}$ with $\mathscr{E}\mathbf{u}$). We can then construct a periodic solution to $(D(\alpha)-\mathbf{k})\mathbf{v}_\mathbf{k} = 0$ for any $\mathbf{k} \in \mathbb{C}$, and in particular for $\mathbf{k} \notin \Gamma^*$, implying, in view of (3.3), that $\alpha \in \mathcal{A}$.

In fact, if $f_\mathbf{k}$ is holomorphic with simple poles at the zeros of $\mathbf{u}$ allowed (we note that the equations $2D_{\bar z}\psi_1 + U(z)\psi_2 = 2D_{\bar z}\psi_2 + U(-z)\psi_1 = 0$ imply that $\partial_{\bar z}^\ell \psi_j(z_S) = 0$ and hence $\mathbf{u} = (z - z_S)\widetilde{\mathbf{u}}$, where $\widetilde{\mathbf{u}}$ is smooth near z_S) then

$$(D(\alpha) - \mathbf{k})\mathbf{v}_\mathbf{k} = 0, \quad \mathbf{v}_\mathbf{k}(z) = e^{\frac{i}{2}(z\bar{\mathbf{k}} + \bar z\mathbf{k})} f_\mathbf{k}(z)\mathbf{v}(z).$$

To obtain periodicity we need

$$\begin{gathered} f_\mathbf{k}(z + \mathbf{a}) = e^{-\frac{i}{2}(\mathbf{a}\bar{\mathbf{k}} + \bar{\mathbf{a}}\mathbf{k})} f_\mathbf{k}(z), \quad \mathbf{a} \in \Gamma, \quad \tfrac{1}{2}(\mathbf{a}\bar{\mathbf{k}} + \bar{\mathbf{a}}\mathbf{k}) = 2\pi(a_1k_1 + a_2k_2), \\ \mathbf{a} = 4\pi(a_1 i\omega + a_2 i\omega^2), \quad \mathbf{k} = \tfrac{1}{\sqrt{3}}(k_1\omega^2 - k_2\omega). \end{gathered}$$

But now, (3.7)–(3.9) show that we can take

$$f_\mathbf{k}(z) = \frac{\theta_{-\frac{1}{6}+k_1/3, \frac{1}{6}-k_2/3}(3z/4\pi i\omega|\omega)}{\theta_{-\frac{1}{6},\frac{1}{6}}(3z/4\pi i\omega|\omega)}. \qquad \square$$

Proof of Theorem 2. The lack of dependence of the spectrum of $T_\mathbf{k}$ on $\mathbf{k} \notin \Gamma^*$ and equivalence of statements (1) and (2) are the content of Proposition 3.1. The definition of $H_\mathbf{k}(\alpha)$ in (1.4) immediately shows their equivalence to statement (3). $\square$

Proof of Theorem 1. In Proposition 3.1 we already obtained a (real) analytic family $\alpha \mapsto \mathbf{u}(\alpha)$. Then $v(\alpha) = W(\mathbf{u}(\alpha), \mathscr{E}\mathbf{u}(\alpha))$ and the equivalence of $v(\alpha)$ to (1) in Theorem 2 follows from Proposition 3.3 and 3.4. $\square$

Remarks. 1. The zero of $\mathbf{u}(\alpha) \in \ker_{L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma, \mathbb{C}^2)} D(\alpha)$ seems to occur at z_S only – see Figure 5. This is also suggested by the following argument: from $v(\alpha) = 0$ we see that $\mathscr{E}\mathbf{u}(z) = f(z)\mathbf{u}(z)$, where, using $v(\alpha) = 0$ again,

$$f(z) := \frac{\psi_2(-z)}{\psi_1(z)} = -\frac{\psi_1(-z)}{\psi_2(z)} = \frac{\alpha U(z)\psi_1(-z)}{2D_{\bar z}\psi(z)}, \tag{3.11}$$

is holomorphic away from $\psi_1^{-1}(0) \cap (D_{\bar z}\psi_1)^{-1}(0)$. We also see that f is meromorphic: in fact, near any point z_0, $\psi_1(z_0 + \zeta) = F_1(\zeta, \bar\zeta)$, $\psi_2(-z_0 - \zeta) = F_2(\zeta, \bar\zeta)$, where $F_j : B_{\mathbb{C}^2}(0, \delta) \to \mathbb{C}$ are holomorphic functions (this follows from real analyticity of

ψ_j, which follows in turn from the ellipticity of the equation – see [HöI, Theorem 8.6.1]). The definition of f and the fact that $\partial_{\bar z} f = 0$ away from zeros of ψ_1 shows that $F_2(\zeta,\xi) = f(z_0+\zeta)F_1(\zeta,\xi)$. We can then choose ξ_0 such that $F_1(\zeta,\xi_0)$ is not identically zero (if no such ξ_0 existed, $\psi_1 \equiv 0$, and hence, from the equation, $\mathbf{u} \equiv 0$). But then $\zeta \mapsto f(z_0+\zeta) = F_2(\zeta,\xi_0)/F_1(\zeta,\xi_0)$ is meromorphic near $\zeta = 0$ and, as z_0 was arbitrary, everywhere. In addition,

$$f(z+\mathbf{a}) = \omega^{-a_1-a_2} f(z), \quad \mathbf{a} \in \Gamma_3, \quad f(\omega z) = f(z), \quad f(z)f(-z) = -1.$$

These symmetries also show that $f(z_S + \omega\zeta) = \omega^{-1} f(z_S+\zeta)$, which means that $f(z_S+\zeta) = \sum_{k\geq k_0} \zeta^{-1+3k} f_k$ and $f(-z_S-\zeta) = \sum_{\ell \geq 1-k_0} \zeta^{-2+3\ell} g_\ell$, for some $k_0 \in \mathbb{Z}$. Hence, if f has only poles of order 1, we have $\mathbf{u}(\alpha, z_S) = 0$. We formulate this bold guess as follows:

$$\mathbf{u}(\alpha) \in \ker_{L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma,\mathbb{C}^2)} D(\alpha), \quad \mathbf{u}(\alpha) \not\equiv 0 \implies \mathbf{u}(\alpha, z) \neq 0, \quad z \notin z_S + \Gamma_3. \tag{3.12}$$

This is related to the following fact, which seems to hold as well:

$$\dim \ker_{L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma,\mathbb{C}^2)} D(\alpha) = 1, \quad \alpha \in \mathbb{C}. \tag{3.13}$$

Proof of (3.12) $\Rightarrow$ (3.13). Suppose that $\mathbf{u} = (\psi_1,\psi_2)^t$ and $\mathbf{v} = (\varphi_1,\varphi_2)^t$ are two elements of the kernel in $L^2_{\rho_{1,0}}$. We then define the (constant) Wronskian $w := \psi_1\varphi_2 - \psi_2\varphi_1$. Since $\varphi_2(\pm z_S) = \psi_2(\pm z_S) = 0$ (see (3.10)), we have $w = 0$ and hence $\mathbf{v} = g\mathbf{u}$, where $g(z) = \varphi_1(z)/\psi_1(z)$. As in the discussion of f given after (3.11), we see that $g(z)$ is a meromorphic function periodic with respect to Γ_3. From (3.12) applied to ψ_1 we see that g can only have poles at $z_S + \Gamma_3$, and applied to $\varphi_1(z)$ we see that g can only have zeros at the same place. But this implies that g is constant. $\square$

2. The elements of the kernel of $D(\alpha) - \mathbf{k}$ can be obtained from the (finite rank) residue of the operator (3.5), and theta functions are already implicitly present there. On one hand (see §5) the operator $(2D_{\bar z} - \mathbf{k})^{-1}$ can be described using Fourier expansion, but on the other hand it can be represented using theta functions: it is the convolution with the fundamental solution of $2D_{\bar z} - \mathbf{k}$ on $\mathbb{C}/\Gamma$. To obtain the convolution kernel (in a construction which works for any torus) we seek a function $G_{\mathbf{k}}$ such that

$$\begin{gathered}(2D_{\bar z} - \mathbf{k})G_{\mathbf{k}} = \delta_0(z), \quad G_{\mathbf{k}} = e^{\frac{i}{2}(\mathbf{k}\bar z + \bar{\mathbf{k}} z)} g_{\mathbf{k}}(z), \quad \partial_{\bar z} g_{\mathbf{k}}|_{\mathbb{C}\setminus\Gamma} = 0, \\ g_{\mathbf{k}}(z+\mathbf{a}) = e^{-\frac{i}{2}(\bar{\mathbf{k}}\mathbf{a} + \mathbf{k}\bar{\mathbf{a}})} g_{\mathbf{k}}(z), \quad \operatorname{Res}_{z=w} g_{\mathbf{k}}(z) = \begin{cases} i/(2\pi), & w \in \Gamma; \\ 0, & w \notin \Gamma. \end{cases}\end{gathered}$$

(The last condition gives $2D_{\bar z} g_{\mathbf{k}}(z) = \sum_{\mathbf{a}\in\Gamma} \delta_{\mathbf{a}}(z)$, as $\partial_{\bar z}(1/(\pi z)) = \delta_0(z)$.)

To find $g_{\mathbf{k}}$ we return to (3.7) and (3.8) and choose

$$\tau' = 4\pi i \omega, \quad \tau\tau' = 4\pi i \omega^2, \quad a = \tfrac{1}{2}, \quad b = \tfrac{1}{2}, \quad a' = \tfrac{1}{2} - k_1, \quad b' = \tfrac{1}{2} + k_2.$$

Hence we have

$$\begin{gathered} g_{\mathbf{k}}(z) := \frac{e^{-\pi i k_1^2 + 2\pi i k_1(\frac12 + k_2)} \theta'_{\frac12,\frac12}(0|\omega)}{2\pi i \theta_{\frac12,\frac12}(\omega k_1 + k_2)|\omega)} \frac{\theta_{\frac12 - k_1, \frac12 + k_2}(z/4\pi i\omega|\omega)}{\theta_{\frac12,\frac12}(z/4\pi i \omega|\omega)}, \\ \mathbf{k} = \tfrac{1}{\sqrt3}(k_1\omega - k_2\omega^2), \quad (k_1,k_2) \notin \mathbb{Z}^2. \end{gathered} \tag{3.14}$$

It would be interesting to derive (1.8) from (3.5) and (3.14). □

3.3. **Existence of magic α's.** We now give a proof of Theorem 3 which amounts to calculating $\operatorname{tr} T_{\mathbf{k}}^4$. For that it is convenient to switch to rectangular coordinates, which are also used in numerical computations (see §5): $z = x_1 + ix_2 = 2i\omega y_1 + 2i\omega^2 y_2$. We have $U(z) = e^{-i(y_1+y_2)} + \omega e^{i(2y_1 - y_2)} + \omega^2 e^{i(-y_1+2y_2)}$ and $2D_{\bar z} = D_{x_1} + iD_{x_2} = (\omega^2 D_{y_1} - \omega D_{y_2})/\sqrt3$. We are then studying

$$\begin{gathered} D_{\mathbf{k}}(\alpha) := D(\alpha) + \mathbf{k} = \tfrac{1}{\sqrt3}\begin{pmatrix} \mathscr{D}_{\mathbf{k}} & \alpha \mathscr{V}(y) \\ \alpha\mathscr{V}(-y) & \mathscr{D}_{\mathbf{k}} \end{pmatrix}, \\ \mathscr{D}_{\mathbf{k}} := \omega^2(D_{y_1} + k_1) - \omega(D_{y_2} + k_2), \\ \mathscr{V}(y) := \sqrt3(e^{-i(y_1+y_2)} + \omega e^{i(2y_1-y_2)} + \omega^2 e^{i(-y_1+2y_2)}), \end{gathered} \tag{3.15}$$

with *periodic* periodic boundary conditions (for $y \mapsto y + 2\pi\mathbf{n}$, $\mathbf{n} \in \mathbb{Z}^2$). In the following, we shall write $\mathscr{V}_\pm(y) := \mathscr{V}(\pm y)$. The operator $T_{\mathbf{k}}$, $\mathbf{k} = (\omega^2 k_1 - \omega k_2)/\sqrt3$, $(k_1,k_2)\notin\mathbb{Z}^2$, is given by

$$T_{\mathbf{k}} := \begin{pmatrix} 0 & \mathscr{D}_{\mathbf{k}}^{-1}\mathscr{V}_+ \\ \mathscr{D}_{\mathbf{k}}^{-1}\mathscr{V}_- & 0 \end{pmatrix}.$$

In this notation,

$$\operatorname{tr} T_{\mathbf{k}}^4 = 18 \operatorname{tr} A^2, \quad A := A_{\mathbf{k}} := \tfrac13 \mathscr{D}_{\mathbf{k}}^{-1}\mathscr{V}_+ \mathscr{D}_{\mathbf{k}}^{-1}\mathscr{V}_-, \tag{3.16}$$

where we note that A^2, a pseudodifferential operator of order -4, is of trace class (see for instance [DyZw19, Theorem B.21]).

By taking the (discrete) Fourier transform on $\mathbb{R}^2/2\pi\mathbb{Z}^2$ we consider the operator $D_{\mathbf{k}}(\alpha)$ as acting on $\ell^2(\mathbb{Z}) \otimes \ell^2(\mathbb{Z})$. With $D := \operatorname{diag}(\ell)_{\ell\in\mathbb{Z}}$ and $J((a_n)_{n\in\mathbb{Z}})) = (a_{n+1})_{n\in\mathbb{Z}}$, we have

$$\begin{gathered} \mathscr{D}_{\mathbf{k}} = \omega^2(D + k_1)\otimes I - \omega I \otimes (D + k_2 I), \\ \mathscr{V}_+/\sqrt3 = J\otimes J + \omega\, J^{-2}\otimes J + \omega^2 J \otimes J^{-2}, \\ \mathscr{V}_-/\sqrt3 = J^{-1}\otimes J^{-1} + \omega J^2 \otimes J^{-1} + \omega^2\, J^{-1}\otimes J^2. \end{gathered} \tag{3.17}$$

The numerical value in Theorem 3 will come from the following, surely classical, computation:

Lemma 3.5. *For* $\Gamma := \omega\mathbb{Z} \oplus \mathbb{Z}$, $\omega := e^{2\pi i/3}$ *and* $\gamma_0 \in \Gamma \setminus \{0\}$ *define*

$$K(\gamma_0) := \sum_{\gamma \in \Gamma \setminus \{0,\gamma_0\}} \gamma^{-2}(\gamma - \gamma_0)^{-2}. \tag{3.18}$$

Then

$$K(\omega m + n) = -\frac{4\pi i(\omega(2n - m) + n + m)}{3(\omega m + n)^3}. \tag{3.19}$$

Proof. We notice that $K(\omega\gamma_0) = \bar{\omega}K(\gamma_0)$. Hence it is enough to evaluate

$$g(\gamma_0) := \sum_{j=0}^{2} \omega^j K(\omega^j \gamma_0) = 3K(\gamma_0). \tag{3.20}$$

Also, if we define $F(z, \gamma_0) := \sum_{\gamma \in \Gamma}(\gamma - z)^{-2}(\gamma - \gamma_0 - z)^{-2}$, then F is a meromorphic Γ-periodic function with the singularity at $z = 0$ given by $2/(z\gamma_0)^2$. Hence,

$$F(z, \gamma_0) = 2\gamma_0^{-2}\wp(z) + K(\gamma_0), \quad \wp(z) := \sum_{\gamma \in \Gamma}\left(\frac{1}{(\gamma - z)^2} - \frac{1 - \delta_{\gamma,0}}{\gamma^2}\right).$$

Using the partial fraction expansion, the fact that $\sum_{j=0}^{2}\omega^j = 0$ and the above series for the $\wp$-function, we obtain

$$\begin{aligned} g(\gamma_0) &= \sum_{j=0}^{2}\omega^j F(z, \omega^j\gamma_0) = \gamma_0^{-2}\sum_{\gamma\in\Gamma}\sum_{j=0}^{2}\bar{\omega}^j\left(\frac{1}{(\gamma - \omega^j\gamma_0 - z)^2} - \frac{2\bar{\omega}^j}{\gamma_0}\frac{1}{(\gamma - \omega^j\gamma_0 - z)}\right) \\ &= \gamma_0^{-2}\sum_{j=0}^{2}\bar{\omega}^j\wp(z) + \sum_{\gamma\in\Gamma}\sum_{j=0}^{2}\frac{\bar{\omega}^j}{\gamma_0^2}\frac{1 - \delta_{\gamma,\omega^j\gamma_0}}{(\gamma - \omega^j\gamma_0)^2} - \sum_{\gamma\in\Gamma}\sum_{j=0}^{2}\frac{2\omega^j}{\gamma_0^3}\frac{1}{(\gamma - \omega^j\gamma_0 - z)}, \end{aligned}$$

where the first term on the right hand side vanishes and both series converge absolutely (this can be checked by taking a common denominator using $\prod_{j=0}^{2}(\zeta - \omega^j\gamma_0) = \zeta^3 - \gamma_0^2$). We now have

$$\begin{aligned} \sum_{\gamma\in\Gamma}\sum_{j=0}^{2}\bar{\omega}^j\frac{1 - \delta_{\gamma,\omega^j\gamma_0}}{(\gamma - \omega^j\gamma_0)^2} &= \lim_{N\to\infty}\sum_{j=0}^{2}\bar{\omega}^j\sum_{|\gamma - \omega^j\gamma_0|\le N}(1 - \delta_{\gamma,0})\gamma^{-2} \\ &= \mathcal{O}(1)\lim_{N\to\infty}\sum_{N - |\gamma_0| \le |\gamma| \le N + |\gamma_0|} N^{-2} = 0. \end{aligned}$$

Hence, using the fact that $\sum_{n\in\mathbb{Z}}((n - a)^{-1} - (n - b)^{-1}) = \pi\cot\pi b - \pi\cot\pi a$,

$$g(\gamma_0) = 2\pi\gamma_0^{-3}\lim_{M\to\infty}\sum_{m=-M}^{M}\sum_{j=0}^{2}\omega^j\left(\cot\pi(m\omega + \omega^j\gamma_0 + z) - \cot\pi(m\omega + z)\right). \tag{3.21}$$

Since $\cot \pi x - \cot \pi y = 2i((e^{2\pi i x} - 1)^{-1} - (e^{2\pi i y} - 1)^{-1})$, $e^{2\pi i n \omega} = (-1)^n e^{-n\pi\sqrt{3}}$, $n \in \mathbb{Z}$, we obtain, with $a_m := (e^{2\pi i(m\omega+z)} - 1)^{-1}$,

$$
\begin{aligned}
&\sum_{m=-M}^{M} (\cot((m+m_0)\omega + n_0 - z) - \cot \pi(m\omega - z)) \\
&\qquad = 2i \sum_{m=-M}^{M} (a_{m+m_0} - a_m) = 2i \sum_{m=M+1}^{M+m_0} a_m - 2i \sum_{m=-M}^{-M+m_0+1} a_m \\
&\qquad = 2i \sum_{m=M+1}^{M+m_0} (-1 + \mathcal{O}(e^{-M})) - 2i \sum_{m=M-m_0+1}^{M} \mathcal{O}(e^{-M}) = -2im_0 + \mathcal{O}(e^{-M}).
\end{aligned}
$$

Inserting this in (3.21) with $\gamma = \omega m_0 + n_0$ (and calculating the corresponding $\omega^j \gamma$) gives

$$
g(\omega m_0 + n_0) = -4\pi i(\omega m_0 + n_0)^{-3}(\omega(2n_0 - m_0) + n_0 + m_0),
$$

which, in view of (3.20), proves (3.19). □

We can now give the

Proof of Theorem 3. To simplify calculations we introduce the following notation:

$$
J^{p,q} := J^p \otimes J^q, \quad p, q \in \mathbb{Z}. \tag{3.22}
$$

Also, for a diagonal matrix $\Lambda = (\Lambda_{ij})_{i,j\in\mathbb{Z}}$ acting on $\ell^2(\mathbb{Z}) \otimes \ell^2(\mathbb{Z})$ we define a new diagonal matrix with the following basic properties:

$$
\begin{gathered}
\Lambda_{p,q} := (\Lambda_{i+p,j+q})_{i,j\in\mathbb{Z}}, \\
(\Lambda\Lambda')_{p,q} = \Lambda_{p,q}\Lambda'_{p,q}, \qquad (\Lambda_{p',q'})_{p,q} = \Lambda_{p+p',q+q'},
\end{gathered} \tag{3.23}
$$

where Λ' is just another diagonal matrix. To express powers of A in (3.16) we will use the following simple fact:

$$
J^{p,q}\Lambda J^{p',q'} = \Lambda_{p,q} J^{p+p',q+q'} = J^{p+p',q+q'}\Lambda_{-p',-q'}. \tag{3.24}
$$

If we put

$$
\Lambda := D_{\mathbf{k}}^{-1}, \quad \Lambda_{mn} = (\omega^2(m+k_1) - \omega(n+k_2))^{-1}, \quad (k_1,k_2) \notin \mathbb{Z}^2,
$$

then, in the notation of (3.16),

$$
\begin{aligned}
A &= \Lambda(J^{1,1} + \omega J^{-2,1} + \omega^2 J^{1,-2})\Lambda(J^{-1,-1} + \omega J^{2,-1} + \omega^2 J^{-1,2}) \\
&= \Lambda\Lambda_{1,1} + \omega\Lambda\Lambda_{1,-2} + \omega^2\Lambda\Lambda_{-2,1} + \omega\Lambda\Lambda_{1,1}J^{3,0} + \omega^2\Lambda\Lambda_{1,1}J^{0,3} \\
&\quad + \omega\Lambda\Lambda_{-2,1}J^{-3,0} + \omega^2\Lambda\Lambda_{1,-2}J^{0,-3} + \Lambda\Lambda_{-2,1}J^{-3,3} + \Lambda\Lambda_{1,-2}J^{3,-3}.
\end{aligned}
$$

The diagonal part of A^2 is then given by (note that the matrices are diagonal and commute)

$$\begin{aligned} B := {} & \Lambda^2\Lambda_{1,1}^2 + \omega^2\Lambda^2\Lambda_{1,-2}^2 + \omega\Lambda^2\Lambda_{-2,1}^2 + 2\omega\Lambda^2\Lambda_{1,1}\Lambda_{1,-2} + 2\omega^2\Lambda^2\Lambda_{1,1}\Lambda_{-2,1} \\ & + 2\Lambda^2\Lambda_{-2,1}\Lambda_{1,-2} + \omega^2\Lambda_{1,1}^2\Lambda\Lambda_{3,0} + \omega^2\Lambda_{-2,1}^2\Lambda\Lambda_{-3,0} + \omega\Lambda_{1,1}^2\Lambda\Lambda_{0,3} \\ & + \omega\Lambda_{1,-2}^2\Lambda\Lambda_{0,-3} + \Lambda_{-2,1}^2\Lambda\Lambda_{-3,3} + \Lambda_{1,-2}^2\Lambda\Lambda_{3,-3}. \end{aligned} \tag{3.25}$$

Since $\operatorname{tr}\Lambda_{k,\ell}^2\Lambda_{p,q}\Lambda_{p',q'} = \operatorname{tr}\Lambda_{k+r,\ell+s}^2\Lambda_{p+r,q+s}\Lambda_{p'+r,q'+s}$, we have

$$\begin{aligned} \operatorname{tr} A^2 = {} & \operatorname{tr}\Lambda^2(\Lambda_{1,1}^2 + 2\Lambda_{-2,1}\Lambda_{1,-2} + 2\Lambda_{2,-1}\Lambda_{-1,2}) \\ & + \omega\operatorname{tr}\Lambda^2(\Lambda_{-2,1}^2 + 2\Lambda_{1,1}\Lambda_{1,-2} + 2\Lambda_{-1,2}\Lambda_{-1,-1}) \\ & + \omega^2\operatorname{tr}\Lambda^2(\Lambda_{1,-2}^2 + 2\Lambda_{1,1}\Lambda_{-2,1} + 2\Lambda_{-1,-1}\Lambda_{2,-1}). \end{aligned}$$

We now find that

$$\Lambda_{\pm2,\mp1}\Lambda_{\mp1,\pm2} + \omega\Lambda_{\mp1,\pm2}\Lambda_{\mp1,\mp1} + \omega^2\Lambda_{\mp1,\mp1}\Lambda_{\pm2,\pm1} = 0.$$

In fact, using

$$\frac{1}{ab} + \frac{1}{bc} + \frac{1}{ca} = \frac{a+b+c}{abc}$$

it suffices to show, say for the $+$ case, that for all $n \in \mathbb{Z}^2$

$$\omega(\Lambda_{2,-1})_{n,n}^{-1} + \bar\omega(\Lambda_{-1,2})_{n,n}^{-1} + (\Lambda_{-1,-1})_{n,n}^{-1} = 0$$

which follows from a direct computation. Hence, the expression for the trace simplifies further to

$$\operatorname{tr} A^2 = \operatorname{tr}\Lambda^2(\Lambda_{1,1}^2 + \omega\Lambda_{-2,1}^2 + \omega^2\Lambda_{1,-2}^2), \tag{3.26}$$

and this expression can be calculated using Lemma 3.5. The singular terms of the sum in (3.26) cancel, as the proof of Lemma 3.5 shows, so we can remove them, and put $k_1 = k_2 = 0$. Noting that $\omega^2 m - \omega n = \omega\gamma$, $\gamma = \omega m - n$, and $\omega^2(m+p) - \omega(n+q) = \omega(\gamma - \gamma_0)$, $\gamma_0 = -\omega p + q$,

$$\begin{aligned} \operatorname{tr} A^2 &= \bar\omega K(-\omega+1) + K(2\omega+1) + \omega K(-\omega-2) \\ &= K(2\omega+1) + \omega K(\omega(2\omega+1)) + \omega^2 K(\omega^2(2\omega+1)) = 3K(2\omega+1) \\ &= 4\pi/\sqrt{3}, \end{aligned}$$

where we used (3.19) and (3.20). In view of (3.16), this concludes the proof. $\square$

Remark. Similar arguments can be used to show that $\sum_{\alpha\in\mathcal{A}}\alpha^{-8} = \operatorname{tr} T_{\mathbf{k}}^4 = 740\pi/\sqrt{3}$.

4. Exponential squeezing of bands

Here we prove a more general version of Theorem 4 valid for potentials with symmetries (2.1). Theorem 4 is then obtained as a special case by choosing the potential as in (1.2). As mentioned in the introduction, in order to see exponential squeezing of bands as $\alpha \to \infty$ for general potentials, it is necessary to impose an additional non-degeneracy assumption.

To introduce our class of potentials, let

$$f_n(z) = f_n(z, \bar{z}) := \sum_{k=0}^{2} \omega^k e^{\frac{n}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}, \quad n \in \mathbb{Z}. \tag{4.1}$$

Then $f_n(\omega z) = \omega f_n(z)$ and

$$f_n(z + \mathbf{a}) = \bar{\omega}^n f_n(z), \quad \mathbf{a} = \tfrac{4}{3}\pi i \omega^\ell, \ \ell = 1, 2.$$

Hence, f_n satisfies (2.1) only when $n \equiv 1 \bmod 3$. We shall therefore consider potentials given by

$$U(z) = U(z, \bar{z}) = \sum_{n \in 3\mathbb{Z}+1} a_n f_n(z, \bar{z}), \quad |a_n| \le c_0 e^{-c_1 |n|}, \tag{4.2}$$

for some constants $c_0, c_1 > 0$. The condition on a_n is equivalent to real analyticity of U.

Special cases of this type of potential have appeared in [GuWa19] and [WaGu19], where the strength of the potential at certain points based on orbital positions and shapes is taken into account to obtain a model different from (1.2) that still satisfies the desired symmetries. Note that the potential in (1.2) is obtained from (4.2) by taking $a_1 = 1$ and $a_n = 0$ for all $n \neq 1$. The potential U_μ appearing in Figure 2 is obtained by taking $a_1 = 1$, $a_{-2} = \mu$ and $a_n = 0$ for $n \neq 1, -2$.

Since $\overline{f_n(\bar{z})} = f_n(z)$ for all n, the symmetry relation $\overline{U(\bar{z})} = U(z)$ (used in Proposition 3.2 to achieve $\mathcal{A} = \overline{\mathcal{A}}$) is equivalent to $\operatorname{Im} a_n = 0$ for all n.

We now impose a generic non-degeneracy assumption that

$$\sum_{n \in 3\mathbb{Z}+1} n \operatorname{Re}(a_n) \neq 0. \tag{4.3}$$

This is trivially satisfied by the standard potential in (1.2), and for the potential U_μ appearing in Figure 2 it holds as long as $\mu \neq \frac{1}{2}$. For such potentials we have the following strengthened version of Theorem 4.

Theorem 5. *Suppose that $H_{\mathbf{k}}(\alpha)$ is given by (1.1) and (1.4) with U given by (4.2) and that*

$$\operatorname{Spec}_{L^2(\mathbb{C}/\Gamma)} H_{\mathbf{k}}(\alpha) = \{E_j(\mathbf{k}, \alpha)\}_{j \in \mathbb{Z}}, \quad E_j(\mathbf{k}, \alpha) \le E_{j+1}(\mathbf{k}, \alpha), \quad \mathbf{k} \in \mathbb{C}, \quad \alpha > 0,$$

with the convention that $E_0(\mathbf{k},\alpha) = \min_j |E_j(\mathbf{k},\alpha)|$. *If* U *satisfies* (4.3)*, then there exist positive constants* c_0*,* c_1*, and* c_2 *such that for all* $\mathbf{k} \in \mathbb{C}$*,*

$$|E_j(\mathbf{k},\alpha)| \le c_0 e^{-c_1\alpha}, \quad |j| \le c_2\alpha, \quad \alpha > 0.$$

Remark. If in (4.2) we assumed instead that $|a_n| \le C_N|n|^{-N}$ for all N, that is, that the potential is *smooth*, then the conclusion would be replaced by $|E_j(\mathbf{k},\alpha)| \le C_N\alpha^{-N}$ for any N. That follows essentially from Hörmander's original argument – see [DSZ04, Theorem 2] and references given there.

To prove Theorem 5 it is natural to consider $h = 1/\alpha$ as a semiclassical parameter. This means that

$$H_{\mathbf{k}}(\alpha) = h^{-1}\begin{pmatrix} 0 & P(h)^* - h\bar{\mathbf{k}} \\ P(h) - h\mathbf{k} & 0 \end{pmatrix}, \quad P = P(h) = \begin{pmatrix} 2hD_{\bar z} & U(z) \\ U(-z) & 2hD_{\bar z} \end{pmatrix},$$

where $U(z)$ is a potential given by (4.2) that satisfies (4.3).

The semiclassical principal symbol of $P(h) - h\mathbf{k}$ (see [DyZw19, Proposition E.14]) is given by

$$p(z,\bar z,\bar\zeta) = \begin{pmatrix} 2\bar\zeta & U(z,\bar z) \\ U(-z,-\bar z) & 2\bar\zeta \end{pmatrix}, \tag{4.4}$$

where we use the complex notation $\zeta = \frac{1}{2}(\xi_1 - i\xi_2)$, $z = x_1 + ix_2$. The Poisson bracket can then be expressed as

$$\{a,b\} = \sum_{j=1}^{2} \partial_{\xi_j} a \partial_{x_j} b - \partial_{\xi_j} b \partial_{x_j} a = \partial_\zeta a \partial_z b - \partial_\zeta b \partial_z a + \partial_{\bar\zeta} a \partial_{\bar z} b - \partial_{\bar\zeta} b \partial_{\bar z} a. \tag{4.5}$$

The key fact we will use is the analytic version [DSZ04, Theorem 1.2] of Hörmander's construction based on the bracket condition: suppose that $Q = \sum_{|\alpha|\le m} a_\alpha(x,h)(hD)^\alpha$ is a differential operator such that $x \mapsto a_\alpha(x,h)$ are real analytic near x_0, and let $q(x,\xi)$ be the semiclassical principal symbol of Q. If there exists

$$q(x_0,\xi_0) = 0, \quad \{q,\bar q\}(x_0,\xi_0) \ne 0, \tag{4.6}$$

then there exists a family $v_h \in C_c^\infty(\Omega)$, Ω a neighbourhood of x_0, such that

$$|(h\partial)_x^\alpha Q v_h(x)| \le C_\alpha e^{-c/h}, \quad \|v_h\|_{L^2} = 1, \quad |(h\partial_x)^\alpha v_h(x)| \le C_\alpha e^{-c|x-x_0|^2/h}, \tag{4.7}$$

for some $c > 0$. The formulation is different than in the statement of [DSZ04, Theorem 1.2], but (4.7) follows from the construction in [DSZ04, §3] – see also [HiSj15, §2.8].

We will use this result to obtain

Proposition 4.1. *There exists an open set* $\Omega \subset \mathbb{C}$ *and a constant* c *such that for any* $\mathbf{k} \in \mathbb{C}$ *and* $z_0 \in \Omega$ *there exists a family* $h \mapsto \mathbf{u}_h \in C^\infty(\mathbb{C}/\Gamma;\mathbb{C}^2)$ *such that for* $0 < h < h_0$*,*

$$|(P(h) - h\mathbf{k})\mathbf{u}_h(z)| \le e^{-c/h}, \quad \|\mathbf{u}_h\|_{L^2} = 1, \quad |\mathbf{u}_h(z)| \le e^{-c|z-z_0|^2/h}. \tag{4.8}$$

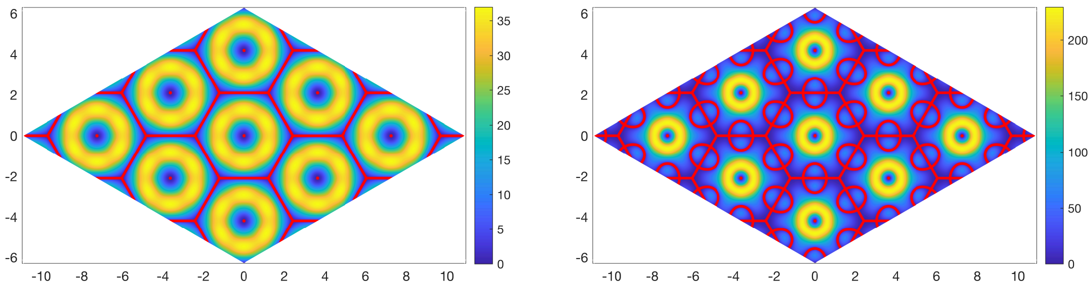

FIGURE 6. A contour plot of $|\{q,\bar{q}\}| = |\operatorname{Im}(\overline{V}^{\frac{1}{2}}\partial_z V)|$ – see (4.9). Here $V(z) = U(z)U(-z)$ with U given by (4.2) so that $U = \sum_n a_n f_n$, $n \equiv 1 \mod 3$. In the left panel, $U = a_1 f_1$ with $a_1 = 1$ so that U coincides with (1.2). In the right panel, $U = a_1 f_1 + a_{-2} f_{-2} + a_4 f_4$ with $a_1 = 1$, $a_{-2} = -0.75$ and $a_4 = 0.15$. The bracket $i\{q,\bar{q}\}$ is non-zero except on a one-dimensional graph and on a set of points given by the red set, and can take any sign by choosing a branch of the square root $V^{\frac{1}{2}}$. The punctured domain around the origin where $|\{q,\bar{q}\}| \neq 0$ is clearly visible.

Proof. To apply (4.7) we reduce to the case of a scalar equation, and for that we look at points where $U(z_0,\bar{z}_0) \neq 0$. In that case, existence of $\mathbf{u}_h$ follows from the existence of $v_h \in C_c^\infty(\Omega';\mathbb{C})$, Ω' a small neighbourhood of z_0 on which $U(z,\bar{z}) \neq 0$, such that

$$Qv_h = \mathcal{O}(e^{-c/h}), \quad v_h(z_0) = 1, \quad |v_h(z)| \leq e^{-c|z-z_0|^2/h},$$
$$Q := U(z,\bar{z})(2hD_{\bar{z}} - h\mathbf{k})\left(U(z,\bar{z})^{-1}(2hD_{\bar{z}} - h\mathbf{k})\right) - U(-z,-\bar{z})U(z,\bar{z}),$$

with estimates for derivatives as in (4.7). We then put

$$\mathbf{u}_h := (v_h, -U(z,\bar{z})^{-1}(2hD_{\bar{z}} - h\mathbf{k})v_h)$$

and normalize to have $\|\mathbf{u}_h\|_{L^2} = 1$. Since such v_h are supported in small neighbourhoods, this defines an element of $C^\infty(\mathbb{C}/\Gamma,\mathbb{C}^2)$. The principal symbol of $2hD_{\bar{z}} - h\mathbf{k}$ is $2\bar{\zeta}$, and basic algebraic properties of the principal symbol map (see [DyZw19, Proposition E.17]) imply that the semiclassical principal symbol of Q is given by

$$q(z,\bar{z},\bar{\zeta}) := \det(p(z,\bar{z},\bar{\zeta})) = 4\bar{\zeta}^2 - V(z,\bar{z}), \quad V(z,\bar{z}) := U(z,\bar{z})U(-z,-\bar{z}).$$

To use (4.7) we need to check Hörmander's bracket condition (4.6): for z in an open neighbourhood of z_0, $U(z_0,\bar{z}_0) \neq 0$, there exists ζ such that

$$q(z,\bar{z},\bar{\zeta}) = 0, \quad \{q,\bar{q}\}(z,\zeta) \neq 0.$$

Since $q = 4\bar{\zeta}^2 - V(z,\bar{z})$, we can take $\zeta = \frac{1}{2}\overline{V}^{\frac{1}{2}}$ (for either branch of the square root) so that, using (4.5),

$$\begin{aligned} i\{q,\bar{q}\} &= i(8\bar{\zeta}\bar{\partial}_z + \partial_z V \partial_\zeta)(4\zeta^2 - \overline{V}) = 8i(\zeta\partial_z V - \overline{\zeta\partial_z V}) \\ &= -16\,\mathrm{Im}(\zeta\partial_z V) = -8\,\mathrm{Im}(\overline{V}^{\frac{1}{2}}\partial_z V). \end{aligned} \tag{4.9}$$

We need to verify that the right-hand side is non-zero at some point z_0, as that will remain valid in an open neighbourhood of z_0.

To do so we write the expression $\mathrm{Im}(\overline{V}^{\frac{1}{2}}\partial_z V)$ from (4.9) as a Taylor series at the origin. With f_n given by (4.1) we observe that $f_n(0) = 0$ for all n, and that

$$\partial_z f_n(0) = \tfrac{n}{2}\sum_{k=0}^{2} e^{\frac{n}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}\Big|_{z=0} = \tfrac{3n}{2}, \qquad \partial_{\bar{z}} f_n(0) = -\tfrac{n}{2}\sum_{k=0}^{2}\omega^{2k} e^{\frac{n}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}\Big|_{z=0} = 0,$$

since $\omega^4 = \omega$ and $1 + \omega + \omega^2 = 0$. Hence,

$$U(z,\bar{z}) = \partial_z U(0) z + O(|z|^2), \qquad \partial_z U(0) = \tfrac{3}{2}\sum_{n=3\mathbb{Z}+1} n a_n. \tag{4.10}$$

Recall that $V(z) = U(z)U(-z)$. Since $U(0) = \partial_{\bar{z}} U(0) = 0$, we have $V(0) = \partial_z V(0) = \partial_{\bar{z}} V(0) = 0$, and

$$\partial_z^2 V(0) = -2(\partial_z U(0))^2, \qquad \partial_z \partial_{\bar{z}} V(0) = \partial_{\bar{z}}^2 V(0) = 0.$$

It follows that

$$V(z) = -z^2(\partial_z U(0))^2(1 + O(|z|)), \qquad \partial_z V(z) = -2z(\partial_z U(0))^2(1 + O(|z|)),$$

which gives

$$\begin{aligned} \overline{V}^{\frac{1}{2}}(z)\partial_z V(z) &= \overline{\sqrt{-z^2(\partial_z U(0))^2}}(-2z(\partial_z U(0))^2)(1 + O(|z|)) \\ &= 2i|z|^2|\partial_z U(0)|^2\partial_z U(0)(1 + O(|z|)). \end{aligned}$$

From this we see that $\mathrm{Im}(\overline{V}^{\frac{1}{2}}\partial_z V) \neq 0$ in a punctured neighbourhood of the origin if $\mathrm{Re}\,\partial_z U(0) \neq 0$, which in view of (4.10) holds by virtue of the non-triviality assumption (4.3). This completes the proof. $\square$

Remark. The open set on which the right-hand side of (4.9) does not vanish can be easily determined numerically, and it is a complement of a one dimensional set – see Figure 6.

To prove Theorem 5 we will use the following fact, with the proof left to the reader:

Proposition 4.2. *Suppose that $g_n \in L^2(\mathbb{C}/\Gamma)$, $n \in \mathbb{Z}^2$, $|n| \leq N$ satisfy $|\langle g_n, g_m\rangle| \leq e^{-M|n-m|^2}$, $\langle g_n, g_n\rangle = 1$. If $M > 3$ then the set $\{g_n\}_{|n|\leq N}$ is linearly independent in $L^2(\mathbb{C}/\Gamma)$.* $\square$

We can now give

Proof of Theorem 5. In the notation of Proposition 4.1, let $C = [a,b] \times [c,d] \Subset \Omega$ and consider the finite set $\mathscr{Z}_h := K\sqrt{h}\mathbb{Z}^2 \cap C$, $|\mathscr{Z}_h| \sim 1/h$. Then (4.8) gives $\mathbf{u}_h^w$, $w \in \mathscr{Z}_h$ (with z_0 replaced by w). Let $M \gg 1$. Using $|w-z|^2 + |w'-z|^2 = \frac{1}{2}|w-w'|^2 + 2|z - \frac{1}{2}(w+w')|^2$, and taking K large enough, we obtain from (4.8)

$$|\langle \mathbf{u}_h^w, \mathbf{u}_h^{w'} \rangle| \leq e^{-M|n-n'|^2}, \quad n := \tfrac{w}{K\sqrt{h}}, \quad n' := \tfrac{w'}{K\sqrt{h}} \in \mathbb{Z}^2, \quad \|\mathbf{u}_h^w\|_{L^2} = 1. \tag{4.11}$$

Abusing notation, let us identify $\mathbf{u}_h^w$ with $(\mathbf{u}_h^w, 0_{\mathbb{C}^2}) \in L^2(\mathbb{C}/\Gamma; \mathbb{C}^4)$, with (4.11) unchanged. We then have

$$\|H_{\mathbf{k}}(\alpha)\mathbf{u}_h^w\|_{L^2(\mathbb{C}/\Gamma)} \leq e^{-c'/h}, \quad h = 1/\alpha. \tag{4.12}$$

Using self-adjointness of $H_{\mathbf{k}}$ and in the notation of Theorem 5, write

$$H_{\mathbf{k}}(\alpha)\mathbf{v} = \sum_{j\in\mathbb{Z}} E_j(\mathbf{k},\alpha)\mathbf{g}_j\langle \mathbf{v}, \mathbf{g}_j\rangle, \quad H_{\mathbf{k}}(\alpha)\mathbf{g}_j = E_j(\mathbf{k},\alpha)\mathbf{g}_j, \quad \langle \mathbf{g}_j, \mathbf{g}_i \rangle = \delta_{ij}.$$

Then (4.12) implies that $\sum_{|E_j(\mathbf{k},\alpha)|\geq e^{-c'/2h}} \mathbf{g}_j \langle \mathbf{u}_h^w, \mathbf{g}_j \rangle = \mathcal{O}(e^{-c'/2h})_{L^2}$, which gives

$$\dim \operatorname{span}\{\mathbf{g}_j\}_{|E_j(\mathbf{k},\alpha)|<e^{-c'/2h}} \geq \dim \operatorname{span}\{\mathbf{u}_h^w\}_{w\in\mathscr{Z}_h}.$$

But (4.11) and Proposition 4.2 show that the right hand side is given by $\mathscr{Z}_h \sim 1/h$. This completes the proof. $\square$

Remark. This simple argument showing exponential squeezing of bands does not apply to the more realistic Bistritzer–MacDonald model of twisted bilayer graphene [BiMa11]. In that case, a more complicated non-self-adjoint system can be extracted from the analogue of $H(\alpha)$, but whenever eigenvalues of the symbol (the analogue of (4.4)), λ, are simple, the Poisson bracket $\{\lambda, \bar{\lambda}\}|_{\lambda=0}$ vanishes [B*21].

5. Numerical results

The results are numerically implemented using rectangular coordinates $z = x_1 + ix_2 = 2i\omega y_1 + 2i\omega^2 y_2$, see §3.3. We then consider

$$H_{\mathbf{k}}(\alpha) = \begin{pmatrix} 0 & D_{\mathbf{k}}(\alpha)^* \\ D_{\mathbf{k}}(\alpha) & 0 \end{pmatrix}, \quad \mathbf{k} = (\omega^2 k_1 - \omega k_2)/\sqrt{3},$$

where $D_{\mathbf{k}}(\alpha)$ is given in (3.15), with*periodic* boundary conditions (for $y \mapsto y + 2\pi\mathbf{n}$, $\mathbf{n} \in \mathbb{Z}^2$). For a fundamental domain in $\mathbf{k}$ we choose $\Omega := \{(k_1,k_2); -\frac{1}{2} \leq k_j < \frac{1}{2}\}$.

5.1. **Numerical implementation.** The discretization is given using a Fourier spectral method; see [Tr00, Chapter 3]. Using the tensor structure of $\mathscr{D}_{\mathbf{k}}$ and $\mathscr{V}$ we start with the standard orthonormal basis of $L^2(\mathbb{R}^2/2\pi\mathbb{Z}^2)$: $e_{\mathbf{n}}(y) := e_{n_1} \otimes e_{n_2}(y) :=$

$e_{n_1}(y_1)e_{n_2}(y_2)$, $e_\ell(t) := (2\pi)^{-\frac{1}{2}}e^{i\ell t}$. Using the identification $[-N,N]\cap\mathbb{Z}\simeq\mathbb{Z}_{2N+1}$, we define

$$\Pi_N : L^2(\mathbb{R}^2/2\pi\mathbb{Z}^2;\mathbb{C}^2)\to\ell^2(\mathbb{Z}^2_{2N+1};\mathbb{C}^2)=\ell^2(\mathbb{Z}_{2N+1};\mathbb{C}^2)\otimes\ell^2(\mathbb{Z}_{2N+1};\mathbb{C}^2),$$
$$\Pi_N\left(\sum_{\mathbf{n}\in\mathbb{Z}^2}a_{\mathbf{n}}e^{i\langle y,\mathbf{n}\rangle}\right)=\{a_{(n_1,n_2)}\}_{|n_j|\le N},\quad a_{\mathbf{n}}\in\mathbb{C}^2,\quad \mathbf{n}=(n_1,n_2)\in\mathbb{Z}^2,$$

and $D^N_{\mathbf{k}}(\alpha):=\Pi_N D_{\mathbf{k}}(\alpha)\Pi_N^*$. Hence,

$$D^N_{\mathbf{k}}(\alpha)=\tfrac{1}{\sqrt{3}}\begin{pmatrix}\mathscr{D}^N_{\mathbf{k}} & \alpha\mathscr{V}^N_+\\ \alpha\mathscr{V}^N_- & \mathscr{D}^N_{\mathbf{k}}\end{pmatrix},$$

where (with $D^N := \operatorname{diag}(\ell)_{-N\le|\ell|\le N}$ and J_N the $2N+1$ dimensional Jordan block)

$$\begin{aligned}
\mathscr{D}^N_{\mathbf{k}} &:= \omega^2(D^N+k_1 I_{\mathbb{C}^{2N+1}})\otimes I_{\mathbb{C}^{2N+1}}-\omega I_{\mathbb{C}^{2N+1}}\otimes(D^N+k_2 I_{\mathbb{C}^{2N+1}}),\\
\mathscr{V}^N_+ &:= \sqrt{3}(J_N\otimes J_N+\omega\,(J_N^2)^t\otimes J_N+\omega^2 J_N\otimes(J_N^2)^t),\\
\mathscr{V}^N_- &:= \sqrt{3}((J_N)^t\otimes(J_N)^t+\omega J_N^2\otimes(J_N)^t+\omega^2\,(J_N)^t\otimes J_N^2).
\end{aligned}$$

The matrix $D^N_{\mathbf{k}}(\alpha)$ has dimension $2(2N+1)^2$. To obtain reasonable accuracy up through the second magic α, one should at least use $N=16$ (giving a matrix of dimension 2,178); for the range $\alpha\in[0,15]$ in Figures 7 and 8, we use $N=96$ (giving dimension 74,498). It is expedient in the former case, and essential in the latter, to use sparse-matrix algorithms that take advantage of the many zero entries in $D^N_{\mathbf{k}}(\alpha)$. To compute the smallest singular values of $D^N_{\mathbf{k}}(\alpha)$, we use Krylov subspace methods, either the inverse Lanczos algorithm adapted from [Tr99, Wr02] or the augmented implicitly restarted Lanczos method [BaRe05] implemented in MATLAB's `svds` command.

Figure 7 shows numerical calculations of the first 41 non-negative eigenvalues of $H_{\mathbf{k}}(\alpha)$. As required by Theorem 4, these eigenvalues decay exponentially, apparently no slower than $e^{-\alpha}$. The vertical lines in the figure indicate the magic α values. We pursue two approaches to locating these magic $\alpha\in\mathcal{A}_{\rm mag}$ (see (1.10) and Theorem 2). The spectral characterization of the set $\mathcal{A}$ of resonant α's via the operator $T_{\mathbf{k}}$ enables the precise calculation of many points in $\mathcal{A}$ as reciprocals of eigenvalues of the discretisation

$$T^N_{\mathbf{k}} := \begin{pmatrix}0 & (\mathscr{D}^N_{\mathbf{k}})^{-1}\mathscr{V}^N_+\\ (\mathscr{D}^N_{\mathbf{k}})^{-1}\mathscr{V}^N_- & 0\end{pmatrix}.$$

To reduce dimensions (and multiplicities) we consider these operators in the decomposition of $L^2(\mathbb{R}/2\pi\mathbb{Z})$ in terms representations of $\Gamma_3/\Gamma\simeq\mathbb{Z}_3^2$ (we did not use the full symmetry group G_3 – see (2.6)). We used this approach to compute Figure 1 and to get initial estimates of the values in Table 1; note however that for large $|\alpha|$ the non-self-adjointness of $T^N_{\mathbf{k}}$ limits the precision to which these eigenvalues can be computed. (This pseudospectral effect is a more significant obstacle to high precision than the errors introduced by truncation to finite N.)

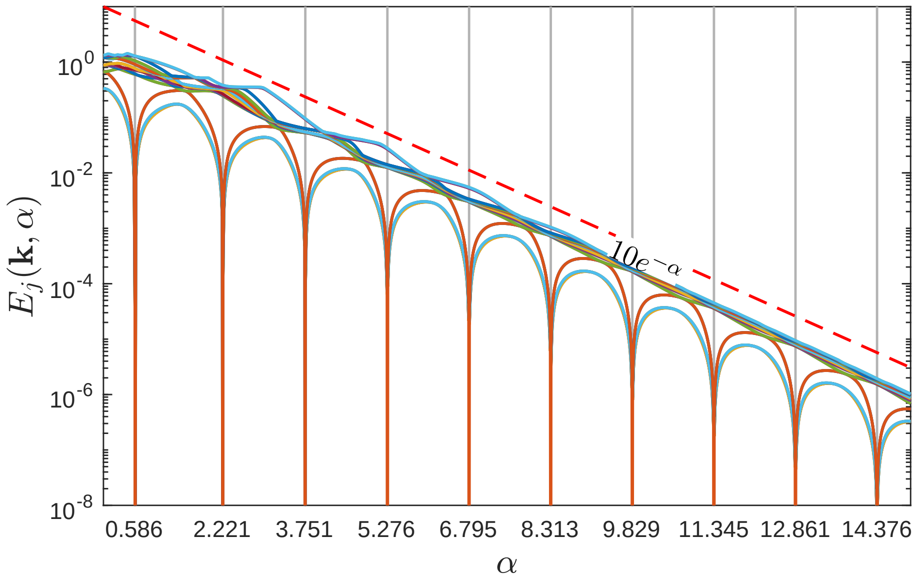

FIGURE 7. Numerical confirmation for Theorem 4: Computed eigenvalues $E_0(\mathbf{k},\alpha)$, ..., $E_{40}(\mathbf{k},\alpha)$ of $H_{\mathbf{k}}(\alpha)$ for $\mathbf{k}_* = 1/(2\sqrt{3}) + i/6$ (see Figure 8). Numerous eigenvalues are quite close together or have high multiplicity.

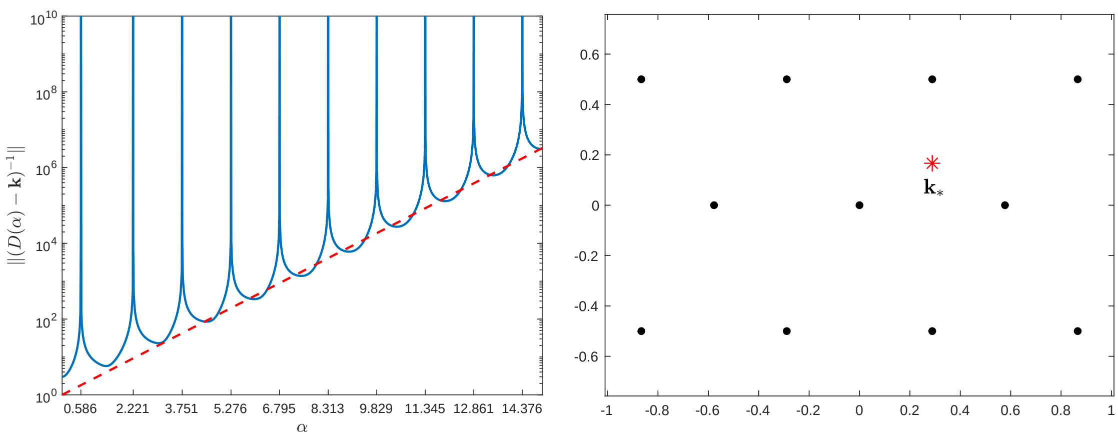

FIGURE 8. On the left, the norm of the resolvent $(D(\alpha)-\mathbf{k})^{-1}$ at $\mathbf{k}_* = 1/(2\sqrt{3}) + i/6$, a point equidistant from three eigenvalues of $D(\alpha)$ for $\alpha \notin \mathcal{A}$. The red dashed line shows e^{α}. The right shows a portion of $\mathrm{S}pec_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \Gamma^*$ for $\alpha \notin \mathcal{A}$.

To understand the accuracy of the values in Table 1, we studied $\|(D^N_{\mathbf{k}}(\alpha))^{-1}\|$ near the putative magic α values. Figure 8 reveals the computational challenge of resolving large magic angles to high fidelity. One can characterize the magic α's as points where $(D(\alpha)-\mathbf{k})^{-1}$ does not exist, and hence they are approximated by α's for which

Table 1. Estimates of the first thirteen magic α's, truncated (not rounded) to digits supported with high confidence by our numerics. The last column shows the difference between consecutive magic α's, which seem to converge a bit above the conjecture of 3/2 in [TKV19].

k	α_k	$\alpha_k - \alpha_{k-1}$
1	0.58566355838955	
2	2.2211821738201	1.6355
3	3.7514055099052	1.5302
4	5.276497782985	1.5251
5	6.79478505720	1.5183
6	8.3129991933	1.5182
7	9.829066969	1.5161
8	11.34534068	1.5163
9	12.8606086	1.5153
10	14.376072	1.5155
11	15.89096	1.5149
12	17.4060	1.5150
13	18.920	1.5147

$\|D_{\mathbf{k}}^N(\alpha)^{-1}\|$ is very large for generic $\mathbf{k}$. Careful scanning for α's around magic values (using $N = 96$ and $N = 128$) refines the estimates and indicates their accuracy. Overall, as α increases $\|D_{\mathbf{k}}^N(\alpha)^{-1}\|$ grows exponentially (as guaranteed by Theorem 4, since $\|D_{\mathbf{k}}^N(\alpha)^{-1}\| = 1/E_0(\mathbf{k}, \alpha)$), so that precisely locating large $\|D_{\mathbf{k}}^N(\alpha)^{-1}\|$ values against this growing background becomes increasingly challenging. Indeed, this numerical struggle nicely parallels the presumed diminishing physical significance of large magic α values (corresponding, as they do, to reciprocals of angles of twisting).

5.2. **Error bounds.** Assuming accuracy of matrix calculations it is possible to give error bounds for the approximation of the actual magic α's. We consider the general situation in which $B \in \mathcal{L}_1(H)$ (a trace class operator on a Hilbert space) is approximated by a $m(N)$-by-$m(N)$ matrix, (in our case $m(N) = (2N + 1)^2$) where

$$B = B_N + E_N, \quad \|E_N\|_1 \leq \rho_1(N)/N^6, \quad \|E_N\| \leq \rho_0(N)/N^8, \tag{5.1}$$

where $\| \bullet \|_1$ and $\| \bullet \|$ are trace class and operator norms, respectively. (The strange look of the estimates is explained by the statement of Proposition 5.2.)

Suppose that the matrix B_N has a simple eigenvalue $\mu_N \in \mathbb{R}$ (computed numerically) and that (by a numerical calculation)

$$\|(B_N - \lambda_j)^{-1}\| \leq C_N^0(\varepsilon), \quad \lambda_j := \mu_N + \varepsilon e^{2\pi i j/J}, \quad j = 0, 1, \cdots, J - 1. \tag{5.2}$$

We then have, for *all* λ with $|\lambda - \mu_N| = \varepsilon$,

$$2\varepsilon C_N^0(\varepsilon)\sin(\pi/2J) < \delta \implies \|(B_N - \lambda)^{-1}\| \leq C_N(\varepsilon) := C_N^0(\varepsilon)(1-\delta)^{-1}. \tag{5.3}$$

We then note that for $|\lambda - \mu_N| = \varepsilon$,

$$\begin{gathered} C_N(\varepsilon)\rho_0(N)/N^8 < \delta \implies (B-\lambda)^{-1} = (B_N - \lambda)^{-1}(I - D_N(\lambda)), \\ D_N(\lambda) := E_N(\lambda)(B_N-\lambda)^{-1}(I + E_N(\lambda)(B_N - \lambda)^{-1})^{-1}, \\ \|D_N(\lambda)\|_1 < C_N(\varepsilon)\rho_1(N)/N^6(1-\delta). \end{gathered} \tag{5.4}$$

These bounds lead to an estimate of the trace class norm: if the assumptions in (5.3), using here the larger constant C_N instead of C_N^0, and (5.4) hold:

$$2\varepsilon C_N(\varepsilon)\sin(\pi/2J) < \delta, \quad C_N(\varepsilon)\rho_0(N)/N^8 < \delta, \tag{5.5}$$

where $\rho_0(N)$ is defined in (5.1) and $C_N(\varepsilon)$ in (5.3), then

$$\|(B-\lambda)^{-1} - (B_N - \lambda)^{-1}\|_1 < C_N(\varepsilon)^2\rho_1(N)/N^6(1-\delta). \tag{5.6}$$

If we define spectral projectors

$$P(\varepsilon) := \frac{1}{2\pi i}\oint_{|\lambda-\mu_N|=\varepsilon}(\lambda - B)^{-1}d\lambda, \quad P_N(\varepsilon) := \frac{1}{2\pi i}\oint_{|\lambda-\mu_N|=\varepsilon}(\lambda - B_N)^{-1}d\lambda, \tag{5.7}$$

we see that if (5.5) holds then

$$\varepsilon C_N(\varepsilon)^2\rho_1(N)/N^6(1-\delta) < 1 \implies \operatorname{tr} P = \operatorname{tr} P_N = 1, \tag{5.8}$$

that is, we have a simple eigenvalue of B within ε of μ_N:

$$|\operatorname{Spec}(B) \cap D(\mu_N, \varepsilon)| = 1. \tag{5.9}$$

If we know that the eigenvalues of B are symmetric with respect to $\mathbb{R}$ it follows that B has a real eigenvalue in $(\mu_N - \varepsilon, \mu_N + \varepsilon)$.

Remark. Anders Hansen pointed it out to us that a similar argument working in greater generality was presented in [Be*15].

We now implement this for the operator $B = B_{\mathbf{k}} = 3A_{\mathbf{k}}$, $\mathbf{k} \notin \Gamma^*$, where $A_{\mathbf{k}}$ is the operator defined in (3.16). The Hilbert space is the symmetry reduced L^2:

$$H = L_0^2(\mathbb{C}/\Gamma) := \{u \in L^2(\mathbb{C}/\Gamma) : u(z+\gamma) = u(z), \gamma \in \Gamma_3/\Gamma\}, \tag{5.10}$$

where $\Gamma_3 = \frac{4}{3}\pi i(\omega\mathbb{Z} \oplus \omega^2\mathbb{Z})$, $\Gamma = 3\Gamma_3$ – see (2.4).

We start with the computation of the constants in (5.1). Let T be a compact operator and $\|T\|_p$ its p-Schatten norm:

$$\|T\|_p = \|T\|_{\mathcal{L}_p(H)} := \left(\sum_{j=0}^{\infty} s_j(T)^p\right)^{\frac{1}{p}}, \quad T \in \mathcal{L}^p(H) \iff \|T\|_p < \infty,$$

where $s_j(T)$ are the singular values of T – see [DyZw19, §B.3]. In the notation of §5.1, we let $\pi_N := I - \Pi_N$. For $p \geq 3$, $M \geq 2$, and $\mathbf{k} = (\omega^2 k_1 - \omega k_2)/\sqrt{3}$, $(k_1, k_2) \in (0,1)^2$, we claim

$$\gamma_p := \sup_{M \geq 2} \frac{\|\pi_M D(\mathbf{k})^{-1}\|_p^p}{(M-1)^{2-p}} \leq \frac{2\pi\, 6^{p/2}}{\sqrt{3}(p-2)}. \tag{5.11}$$

In fact,

$$\begin{aligned}
\|\pi_M D(\mathbf{k})^{-1}\|_p^p &= 3^{p/2} \sum_{|m|>M \vee |n|>M} |(m+k_1) - \omega^2(n+k_2)|^{-p} \\
&\leq 3^{p/2} \sum_{|m|\geq M \vee |n|\geq M} |m^2 + mn + n^2|^{-p/2} \\
&\leq 3^{p/2} \int_{M-1}^{\infty} \int_0^{2\pi} \frac{1}{r^{p-1}(1+\cos(\varphi)\sin(\varphi))^{p/2}}\, d\varphi\, dr \qquad (5.12) \\
&= 3^{p/2} \frac{(M-1)^{2-p}}{p-2} \int_0^{2\pi} \frac{1}{(1+\frac{1}{2}\sin(2\varphi))^{p/2}}\, d\varphi \\
&\leq \frac{2\pi 6^{p/2}}{\sqrt{3}} \frac{(M-1)^{2-p}}{p-2}
\end{aligned}$$

where we used, with $f(\varphi) := (1 + \frac{1}{2}\sin 2\varphi)^{-1/2}$,

$$\|f\|_2^2 = \frac{4\pi}{\sqrt{3}}, \quad \|f\|_\infty = 2^{\frac{1}{2}}, \quad \|f\|_p^p \leq \|f\|_2^2 \|f\|_\infty^{p-2}.$$

(The integral can also be estimated very accurately using the method of steepest descent.) In addition, we observe that for the operator norm and $M \geq 1$,

$$\|\pi_M D(\mathbf{k})^{-1}\| \leq \sqrt{3} \sup_{|m|\geq M \vee |n|\geq M} (m^2 + mn + n^2)^{-\frac{1}{2}} \leq 2/M. \tag{5.13}$$

We used these estimates to compare finite rank operators used in numerical calculations to powers of $T_{\mathbf{k}}^p$:

Proposition 5.1. *In the notation of §5.1, and with $k_1, k_2 \in (-1,1)$, $N \geq 2p \geq 6$, we have*

$$\|T_{\mathbf{k}}^p - \Pi_N T_{\mathbf{k}}^p \Pi_N\|_1 \leq \frac{4\pi 54^{p/2} \rho_1(N,p)}{\sqrt{3}(p-2)N^{p-2}}$$

and in operator norm

$$\|T_{\mathbf{k}}^p - \Pi_N T_{\mathbf{k}}^p \Pi_N\| \leq 6^p 2 \rho_0(N,p) N^{-p},$$

where

$$\rho_j(N,p) = \prod_{\ell=0}^{p-1} (1 - (2\ell + j)/N)^{-1+\frac{2j}{p}}. \tag{5.14}$$

Proof. We first observe that

$$\begin{aligned}\|T_{\mathbf{k}}^p - \Pi_N T_{\mathbf{k}}^p \Pi_N\|_1 &= \|T_{\mathbf{k}}^p - (I-\pi_N)T_{\mathbf{k}}^p + (I-\pi_N)T_{\mathbf{k}}^p\pi_N\|_1 \\ &\le \|\pi_N T_{\mathbf{k}}^p\|_1 + \|T_{\mathbf{k}}^p\pi_N\|_1, \quad \pi_N = I - \Pi_N.\end{aligned}$$

We will estimate the first term, with a same argument applicable to the second term.

Letting $T = T_{\mathbf{k}}$, we write $T = D_{\mathbf{k}}(0)^{-1}V$, where V is the potential with $U(z)$ and $U(-z)$ on the antidiagonal. We note that $\|V\| \le 3$. By analysing the potential in (1.2) we find that

$$\pi_N T = \pi_N T \pi_{N-2}. \tag{5.15}$$

Hence (using Schatten norms)

$$\|\pi_N T^p\|_1 \le \prod_{\ell=0}^{p-1} \|\pi_{N-2\ell} T\|_p \le 3^p \prod_{\ell=0}^{p-1} \|\pi_{N-2\ell} D_{\mathbf{k}}(0)^{-1}\|_p. \tag{5.16}$$

For $M \ge 2$, (5.11) gives

$$\|\pi_M D_{\mathbf{k}}(0)^{-1}\|_p \le \gamma_p^{\frac{1}{p}} (M-1)^{-1+\frac{2}{p}}, \quad p \ge 3, \tag{5.17}$$

and hence we have, using (5.11) and (5.14),

$$\|\pi_N T^p\|_1 \le \frac{2\pi 54^{p/2}\rho_1(N,p)}{\sqrt{3}(p-2)N^{p-2}}.$$

Combined with the same estimate for $\|T^p\pi_N\|_1$ this implies the result. The operator norm estimate is fully analogous, using (5.13). ☐

We recall that $\mathscr{L}_{\mathbf{a}}$ commutes with $D_{\mathbf{k}}(0)$ and V, where V is as in the proof of Proposition 5.1. It also commutes with Π_N since pull backs by translations and multiplication by constants do not change orders of trigonometric polynomials. This gives an action of $\mathbb{Z}_3^2$ on $L^2(\mathbb{C}/\Gamma, \mathbb{C}^2)$ which can then be decomposed using nine irreducible representations of that group (2.8):

$$L^2_{\mathbf{p}}(\mathbb{C}/\Gamma;\mathbb{C}^2) = \{\mathbf{u} \in L^2(\mathbb{C}/\Gamma;\mathbb{C}^2) : \mathscr{L}_{\mathbf{a}}\mathbf{u} = \pi_{\mathbf{p}}(\mathbf{a})\mathbf{u}\},$$

where $\mathbf{p} = (\omega^2 p_1 - \omega p_2)/\sqrt{3}$, $p_j \in \mathbb{Z}_3$, $\pi_{\mathbf{p}}(\mathbf{a}) = \exp(i\,\mathrm{Re}(\mathbf{a}\bar{\mathbf{p}}))$. We then specialize to this symmetry reduced case and power $p = 8$. The former gives a small improvement:

Proposition 5.2. *Suppose that $B = B_{\mathbf{k}} = 3A_{\mathbf{k}}$, $\mathbf{k} = \omega^2/2\sqrt{3}$, where $A_{\mathbf{k}}$ comes from (3.16) and H is given by (5.10). Then, with Π_N given in §5.1, and ρ_j defined in (5.14),*

$$\begin{aligned}&\|B^4 - \Pi_N B^4 \Pi_N\|^{\frac{1}{6}}_{\mathcal{L}_1(L^2_{\mathbf{0}}(\mathbb{C}/\Gamma,\mathbb{C}^2))} \le 10.23 N^{-1}\rho_1(8,N)^{\frac{1}{6}}, \\ &\|B^4 - \Pi_N B^4 \Pi_N\|_{\mathcal{L}(L^2(\mathbb{C}/\Gamma,\mathbb{C}^2))} \le 6^8 2\rho_0(8,N)N^{-8}.\end{aligned} \tag{5.18}$$

Moreover, at every magic angle, $\alpha \in \mathcal{A}$, the Hamiltonian $H(\alpha)$ exhibits at least 18 flat bands.

TABLE 2. The values of N needed to obtain a rigorous error bound of $\delta = 10^{-k}$, as computed using the `guarantee.m` code in the Appendix (using the default `NN=16`). The matrices used in calculations then have size $(2N+1)^2$-by-$(2N+1)^2$. Hence the rigorous error estimates are realistic for α_1 and for rough bounds on α_2 and α_3 but not for higher α_j's. All the values of $N \leq 328$ here were certified by a second (long) run of `guarantee.m` with the procedure described in the Appendix.

k	α_1	α_2	α_3
1	21	128	374
2	21	159	476
3	28	226	689
4	38	328	1011
5	51	472	1480
6	71	691	2168
7	100	1012	
8	145	1485	
9	211		

Proof. We observe that we have unitary equivalence,

$$U_{\mathbf{p}}\mathbf{u}(z) : L^2_{\mathbf{q}}(\mathbb{C}/\Gamma;\mathbb{C}^2) \to L^2_{\mathbf{p}+\mathbf{q}}(\mathbb{C}/\Gamma;\mathbb{C}^2), \quad U_{\mathbf{p}}\mathbf{u}(z) := e^{-i\,\mathrm{Re}(z\bar{\mathbf{p}})}\mathbf{u}(z),$$

and that,

$$U_{\mathbf{p}} T_{\mathbf{k}} U_{\mathbf{p}}^* = T_{\mathbf{k}+\mathbf{p}} = T_{\mathbf{k}}, \quad \mathbf{p} \in \Gamma^*, \quad \mathbf{k} \notin \Gamma^*.$$

Hence, in the computation of the trace class norm on L^2_0 we gain $1/9$ and Proposition 5.1 gives, with H of (5.10) and $p = 8$ (see (3.16): the 8th power of $T_{\mathbf{k}}$ corresponds to the 4th power of B),

$$\|B^4 - \Pi_N B^4 \Pi_N\|^{\frac16}_{\mathcal{L}_1(L^2_{\mathbf{0}}(\mathbb{C}/\Gamma,\mathbb{C}^2))} \leq \left(\frac{4\pi 54^4 \rho_1(8,N)}{54\sqrt{3}}\right)^{\frac16} N^{-1} = 10.2244\, \rho_1(8,N)^{\frac16} N^{-1},$$

which gives the desired estimate. The operator norm is estimated using Proposition 5.1 as there is no gain from symmetry reduction. $\square$

Combining Proposition 5.2 and (5.8) provides an error estimate in the numerical computation of α_1 and α_2. In principle, the same methods are applicable for higher α's shown in Table 1 but that seems to require much larger matrices and any claim of a "rigorous" calculation is not feasible.

Replacing B with B^4 of Proposition 5.2 we see that (5.1) holds for that B. We then have

$$|\beta^{-8} - \alpha_j^{-8}| < \varepsilon := \beta^{-8} - (\beta+\delta)^{-8} \implies |\beta - \alpha_j| < \delta.$$

TABLE 3. Values needed for the backward error calculation guaranteeing 10^{-k} accuracy for computing α_j (those errors are much smaller than those from Proposition 5.2). We show $e_j = \|(B_{N_k^j} - \mu_{32}^j)u_{32}^j\|/\|u_{32}^j\|$ where N_k^j comes from Table 2, μ_{32}^j is the eigenvalue closest to α_j^{-8} obtained using B_{32}, and u_{32}^j is the corresponding eigenvector extended by 0 – see `backerror.m` in the Appendix. These values, on the order of machine precision, can vary slightly based on implementation, machine, and MATLAB version.

k	$e_1 10^{15}$	$e_2 10^{15}$	$e_3 10^{15}$
1		4.33	3.47
2		4.33	3.47
3		4.33	3.47
4	1.68	4.33	3.47
5	1.68	4.33	3.47
6	1.68	4.33	3.47
7	1.68	4.33	
8	1.68	4.33	
9	1.68		

This is particularly favourable in the case of α_1 as then $\beta \simeq 0.5$. (We have to take ε sufficiently small to avoid other eigenvalues of B.)

The method described above is implemented in `BkN.m` in the Appendix, which computes $\Pi_N B_{\mathbf{k}} \Pi_N$ (see Proposition 5.2). The code `guarantee.m` then returns an N for which we obtain an accuracy of δ. We have to trust the numerical calculation of the smallest singular value of $(2N+1)^2$-by-$(2N+1)^2$ matrices needed for (5.2) and (5.3). To estimate the backward error associated with an approximate eigenpair of B_N, we need to calculate $\|(B_N - \mu_N)u_N\|$, where μ_N and u_N are the eigenvalue and eigenvector returned by MATLAB. We know then that μ_N is an *exact* eigenvalue of $B_N + R_N$ where $\|R_N\| \le \|(B_N - \mu_N)u_N\|/\|u_N\|$. In principle R_N should be added to E_N, but those errors are negligible compared to our estimates on E_N. We should stress that, for these estimates, we do not need to calculate μ_N and u_N from B_N for the large values of N given in Table 2. It is sufficient to compute the eigenpair for B_{32}, then take $\mu_N = \mu_{32}$ and build $u_N \in \mathbb{C}^{(2N+1)^2}$ by extending $u_{32} \in \mathbb{C}^{4225}$ by 0s. (This extension is justified by noting that the function approximated by u_N is a solution of an elliptic equation with analytic coefficients, hence analytic [HöI, Theorem 9.5.1]. Consequently, Fourier coefficients decay exponentially.) We show the resulting error in Table 3.

Table 2 gives estimates of values of N for which calculated α's are within $\delta = 10^{-k}$ of the actual elements of $\mathcal{A}_{\mathrm{mag}}$. Table 3 gives the estimates of the deviation of B_N from the matrix with eigenvalues given by a MATLAB calculation. Hence we can claim a rigorous calculation for α_1 and α_2 within errors 10^{-9} and 10^{-3}, respectively.

Appendix

We include a MATLAB code, `BkN.m`, that constructs a sparse matrix of the truncation (as described in §5.1) of the operator of $B_{\mathbf{k}} := 3A_{\mathbf{k}}$ for the potential

$$U_\mu(z) = \sum_{k=0}^{2} \omega^k \left(e^{\frac{1}{2}(\bar z \omega^k - z\bar\omega^k)} + \mu e^{\bar z \omega^k - z \bar\omega^k} \right); \tag{A.1}$$

see Figure 2.

Approximations of real and complex elements of the magic set $\mathcal{A}$ are given by computing the spectrum of $B_{\mathbf{k}}$:

$$\lambda \in \operatorname{Spec}_{L^2_{\mathbf{0}}(\mathbb{C}/\Gamma;\mathbb{C}^2)}(B_{\mathbf{k}}) \implies 1/\sqrt{\lambda} \in \mathcal{A}, \quad \mathbf{k} \notin \Gamma^*. \tag{A.2}$$

To obtain all α's with multiplicities we should consider the action on all representations of Γ_3/Γ rather than just (5.10) – see §2.1 and the proof of Proposition 5.2. For instance, in MATLAB,

$\alpha_1 \simeq$ `real(1./sqrt(eigs(BkN(0.5,8),1))) = 0.585663558389558`.

The size of the matrix is 289-by-289 ($(2N+1)^2 = 289$, $N = 8$) and no improvement is achieved by taking larger matrices.

```
function B = BkN(k,N);    % create Pi_N * Bk * Pi_N
  N0 = N; N=N+2; N2 = N;
  Rp=RR(k,N,1); Rm=RR(k,N,-1);
  omega=exp(2i*pi/3); N=2*N+1; n=N^2;
  J1 = spdiags(ones(N,1),1,N,N);
  Vp = speye(n)+omega^2*kron(speye(N),J1')+omega*kron(J1',speye(N));
  Vm = speye(n)+omega^2*kron(speye(N),J1)+omega*kron(J1,speye(N));
  B = Rp*Vp*Rm*Vm/3;
  indx = downsize(N0,N2);
  B = B(indx,indx);
end
function RR=RR(k,N,j)
  kk=-N:1:N; N=2*N+1; n=N^2; kk1=kk-j/6; kk1=spdiags(kk1',0,N,N);
  omega=exp(2i*pi/3);
  RR = omega^2*kron(kk1,speye(N))-omega*kron(speye(N),kk1);
  RR = RR-(omega^2*real(k)-omega*imag(k))*speye(size(RR));
  RR = spdiags(1./diag(RR),0,n,n);
end
function indx = downsize(N1,N2); % indices to truncate from N1 to N2
 n1 = max(N1,N2); n2 = min(N1,N2); dn = n1-n2;
```

```
 indx = reshape(1:(2*n1+1)^2,2*n1+1,2*n1+1);
 indx = indx(dn+1:dn+2*n2+1,dn+1:dn+2*n2+1);
 indx = reshape(indx,(2*n2+1)^2,1);
end
```

To reproduce (half of) Figure 1 one simply calls

```
plot(1./sqrt(eigs(BkN(0.5,32),800)),'ro','LineWidth',1.5)
xlim([0,18]), ylim([-9,9])
```

The error bounds based on Proposition 5.2 are implemented in `guarantee.m`, which returns an estimate on N needed to obtain accuracy δ using `BkN.m`. The subroutine `Bk4` uses `BkN` to form $\Pi_N B_{\mathbf{k}}^4 \Pi_N$, via (5.15). As explained in §5.2 the only "non-rigorous" aspect here involves the calculation of the smallest singular values of sparse matrices (a reliable numerical task). To find N for, say, accuracy $\delta = 0.1$ for computing α_2, the command `guarantee(0.1,2)` returns an approximation, $N = 128$, based on an estimate of those singular values with a lower N (experimentally, always the same). To have a "rigorous" confirmation, $N = 128$ should then be used to run `guarantee(0.1,2,116)` (which again produces $N = 116$, though at a much longer run time). Table 2 was produced using `guarantee(`10^{-k}`,p)`, $p = 1, 2, 3$. We ran the second refinement step to confirm N for all values in this table with $N \leq 328$.

```
function N = guarantee(delta,p,NN)
% returns N for which alpha_p is computed within error delta, p = 1,2,3
 if (nargin<2) p=1; end
 if (nargin<3) NN=16; end
 alpha(1)=0.585663; alpha(2)=2.221182; alpha(3)=3.7514055;
 rad(1)=72.2;rad(2)=0.0017;rad(3)=2.3830e-05; % dist to the rest of A.^-8
 bet=alpha(p); epsi=bet^-8-(bet+delta)^-8; epsi=min(rad(p)/5,epsi);
 Cep=circle_norm(epsi,NN,bet); M=16; C0=2*6^8*rhoj(M,0)*M^(-8)*Cep;
 while C0>0.5, M = M+1; C0=Cep*2*6^8*rhoj(M,0)*M^(-8); end
 N=M; C0=Cep*(1-C0)^(-1); C1=10.23*rhoj(N,1)^(1/6);
 while (C0*Cep*epsi)^(1/6)*C1 > N, N=N+1; C1=10.23*rhoj(N,1)^(1/6); end
end
function [C,J] = circle_norm(epsi,N,bet)
% Computes the approximate norm of (B-lambda)^-1 for B=Pi_N*Bk(0.5)^4*Pi_N
% and |lambda-mu|=epsi where mu is an approximate eigenvalue of B
 b=1/bet^8; B4=Bk4(0.5,N); J=10; [C1,del]=Jtest(J,B4,epsi,b);
 while del>0.5, J=2*J; [C1,del]=Jtest(J,B4,epsi,b); end
 C=C1/(1-del);end
function [C1,del]=Jtest(J,T,epsi,mu)
% calculates the maximum of the norm of (T-lambda)^{-1}, T sparse
% at J points on the circle |lambda-mu|=epsi
 mu = eigs(T,1,mu);
```

```
 zz = exp(1i*(0:1:J-1)*2*pi/J);   la = mu + epsi*zz;
 for j=1:J, A=T-la(j)*speye(size(T)); CC(j)=1/svds(A,1,'smallest'); end
 C1=max(CC); del=2*max(CC)*epsi*sin(pi/(2*J)); end
function rhoj = rhoj(N,j)
 rhoj=1; for ell=0:7 rhoj=rhoj*(1-(2*ell+j)/N)^(-1+j/4); end
end
function B4 = Bk4(k,N); % create Pi_N * Bk^4 * Pi_N
 Bp8 = BkN(k,N+8);                  % Pi_{N+8} Bk Pi_{N+8}
 Bp4 = BkN(k,N+4);                  % Pi_{N+4} Bk Pi_{N+4}
 Bp8sq = Bp8^2;                     % (Pi_{N+8} Bk Pi_{N+8})^2
 indx_8_4 = downsize(N+4,N+8);
 Bp8sq = Bp8sq(indx_8_4,indx_8_4);  % Pi_{N+4} Bp8sq Pi_{N+4}
 B4    = Bp4*Bp8sq*Bp4;
 indx_4_0 = downsize(N,N+4);
 B4    = B4(indx_4_0,indx_4_0);
end
```

Finally we include the code used to obtain Table 3, using the discretization in `BkN.m`.

```
function ba = backerror(N2,p,N1)
  if (nargin < 3) N1=32; end
  N1 = min(N2-1,N1);
  alpha(1)=0.585663; alpha(2)=2.221182; alpha(3)=3.7514055;
  al = alpha(p); mu = 1/al^8; B1 = BkN(0.5,N1); B2 = BkN(0.5,N2);
  [v1,lam1] = eigs(B1,1,1/al^2);
% inflate the N1 eigenvector to N2 by:
% - shaping it into a (2*N1+1)-by-(2*N1+1) matrix;
% - padding it with a border of dN := N2 - N1 zeros;
% - reshaping it into a (2*N2+1)^2 length vector.
  dN = N2-N1;
  V1 = [zeros(dN,2*N2+1);
        zeros(2*N1+1,dN)  reshape(v1,2*N1+1,2*N1+1) zeros(2*N1+1,dN);
        zeros(dN,2*N2+1)];
  v2 = reshape(V1,(2*N2+1)^2,1); ba = norm(B2*v2-lam1*v2)/norm(v2);
end
```

Acknowledgements. We would like to thank Mike Zaletel for bringing [TKV19] to our attention, Alexis Drouot for helpful discussions, and Michael Hitrik for bringing [Se86] to our attention. SB gratefully acknowledges support by the UK Engineering and Physical Sciences Research Council (EPSRC) grant EP/L016516/1 for the University of Cambridge Centre for Doctoral Training, the Cambridge Centre for Analysis. ME and MZ were partially supported by the National Science Foundation under the grants DMS-1720257 and DMS-1901462, respectively. JW was partially supported by the Swedish Research Council grants 2015-03780 and 2019-04878.

References

[BaRe05] J. Baglama and L. Reichel, *Augmented implicitly restarted Lanczos bidiagonalization methods*, SIAM J. Sci. Comp. **27**, 19–42, 2005.

[B*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*15] J. Ben-Artzi, M.J. Colbrook, A.C Hansen, O. Nevanlinna, M. Seidel, *Computing Spectra – On the Solvability Complexity Index Hierarchy and Towers of Algorithms,* arXiv:1508.03280.

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

[DSZ04] N. Dencker, J. Sjöstrand and M. Zworski, *Pseudospectra of semiclassical differential operators*, Comm. Pure Appl. Math. **57**(2004), 384-415.

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

[GuWa19] F. Guinea and N. R. Walet, *Continuum models for twisted bilayer graphene: effect of lattice deformation and hopping parameters*, Physical Review B, **99**, 205134:1–16, 2019.

[HiSj15] M. Hitrik and J. Sjöstrand, *Two minicourses on analytic microlocal analysis,* in "Algebraic and Analytic Microlocal Analysis", M. Hitrik, D. Tamarkin, B. Tsygan, and S. Zelditch, eds. Springer, 2018, arXiv:1508.00649.

[HöI] L. Hörmander, *The Analysis of Linear Partial Differential Operators I. Distribution Theory and Fourier Analysis,* Springer Verlag, 1983.

[Ka80] T. Kato, *Perturbation Theory for Linear Operators*, Corrected second edition, Springer, Berlin, 1980.

[Mu83] D. Mumford, *Tata Lectures on Theta. I.* Progress in Mathematics, **28**, Birkhäuser, Boston, 1983.

[Se86] R. Seeley, *A simple example of spectral pathology for differential operators,* Comm. PDE, **11**(1986), 595–598.

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

[Tr99] L. N. Trefethen, *Computation of pseudospectra*, Acta Numerica **8** 247–295, 1999.

[Tr00] L. N. Trefethen, *Spectral Methods in MATLAB*, SIAM, Philadelphia, 2000.

[TrEm05] L. N. Trefethen and M. Embree, *Spectra and Pseudospectra: The Behavior of Nonnormal Matrices and Operators*, Princeton University Press, Princeton, 2005.

[WaGu19] N. R. Walet and F. Guinea, *The emergence of one-dimensional channels in marginal-angle twisted bilayer graphene*, 2D Materials, **7** 15–23, 2019.

[WaLu21] A.B. Watson and M. Luskin, *Existence of the first magic angle for the chiral model of bilayer graphene,* arXiv:2104.06499.

[Wr02] T. G. Wright, *EigTool*, software available at `https://github.com/eigtool`, 2000.

E-mail address: `simon.becker@damtp.cam.ac.uk`

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, Cambridge, CB3 0WA, United Kingdom.

E-mail address: `embree@vt.edu`

Department of Mathematics, Virginia Tech, Blacksburg, VA 24061, USA

E-mail address: jens.wittsten@math.lu.se

Centre for Mathematical Sciences, Lund University, Box 118, SE-221 00 Lund, Sweden, and Department of Engineering, University of Borås, SE-501 90 Borås, Sweden

E-mail address: zworski@math.berkeley.edu

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