MATHEMATICS OF MAGIC ANGLES 
IN A MODEL OF TWISTED BILAYER GRAPHENE

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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:

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

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

\[ U(z) = U(z, \bar{z}) := \sum_{k=0}^{2} \omega^k e^{\frac{i}{2}(i\omega^k - \bar{\omega}^k)}, \quad \omega := e^{2\pi i/3}. \]

(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 \( \alpha \) is essentially the reciprocal of

![Figure 1](image_url)

**Figure 1.** Reciprocals of magic angles for the specific potential (1.2): resonant \( \alpha \)'s (red circles) come from the full spectrum of the compact operator (1.7) defining magic angles, and the magic \( \alpha \)'s (black dots) are the reciprocals of the “physically relevant” positive angles.
the angle of twisting between the two layers. The results of this paper are valid for potentials satisfying symmetries (2.1) except for 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 $\Gamma$ (see (2.2) below) and magic angles are defined as the $\alpha$’s (or rather their reciprocals) at which

$$0 \in \bigcap_{k \in \mathbb{C}} \text{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_k(\alpha)), \quad H_k(\alpha) := \begin{pmatrix} D(\alpha) - k & D(\alpha)^* - k \end{pmatrix}. \quad (1.3)$$

The Hamiltonian $H_k(\alpha)$ comes from the Floquet theory of $H(\alpha)$ and (1.3) 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 effects such as superconductivity are expected 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 [BM11] and that is discussed in [B*20].

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

$$W(u, v) = \det[u, v], \quad u, v \in \mathbb{C}^2, \quad (1.4)$$

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

$$\mathcal{E}u(\alpha, z) := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} u(\alpha, -z). \quad (1.5)$$

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 (2.1). Then there exists a real-analytic family (unique up to a multiplicative factor) $\mathbb{R} \ni \alpha \mapsto u(\alpha) \in C^\infty(\mathbb{C}/\Gamma; \mathbb{C}^2)$ such that $u(0) = (1, 0)^t$, $D(\alpha)u(\alpha) = 0$ and, in the notation of (1.3),

$$0 \in \bigcap_{k \in \mathbb{C}} \text{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_k(\alpha)) \iff W(u(\alpha), \mathcal{E}u(\alpha)) = 0,$$

where $W$ is given by (1.4).

A more precise, representation theoretical, description of $u(\alpha)$ will be given in §2. In §3 we show that (after possibly switching $u$ and $\mathcal{E}u$)

$$v(\alpha) := W(u(\alpha), \mathcal{E}u(\alpha)) = 0 \iff u(\alpha, z_S) = 0, \quad z_S := \frac{4\sqrt{3}}{9\pi}$$

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

$$u_k(z) = e^{\frac{1}{2}(z + z_k)} \frac{\theta_{z + \frac{1}{3}} \theta_{z - \frac{1}{3}}}{\theta_{z + \frac{1}{3}}} \frac{e^{\frac{1}{2}(z + e^{i\omega}|\omega|)}}{e^{\frac{1}{2}(z + e^{i\omega}|\omega|)}} u(z), \quad k = \frac{1}{\sqrt{3}}(k_1\omega^2 - k_2\omega), \quad (1.6)$$
Figure 2. For $U_\mu(z) = U(z) + \mu \sum_{k=0}^{2} \omega^k e^{\bar{z} \omega^k - z \omega^k}$, 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 (1.10) can be expected. The coloured paths trace the dynamics of magic $\alpha$’s for $-2.2 \leq \mu \leq -1.7$: to understand the dependence of “physically relevant” real $\alpha$’s complex values should be considered.

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 $\alpha$’s satisfying (1.3). Combined with some symmetry reductions (see §§2,5) this characterization allows a precise calculation of the leading magic $\alpha$’s.

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

$$T_k := (2D_z - k)^{-1} \begin{pmatrix} 0 & U(z) \\ U(-z) & 0 \end{pmatrix}, \quad k \notin \Gamma^*,$$

where $U(z)$ is given by (1.2), or more generally satisfies $U \in C^\infty(\mathbb{C}/\Gamma; \mathbb{C})$ and (2.1). Then the spectrum of $T_k$ is independent of $k \notin \Gamma^*$, and the following statements are equivalent:

\[ \zeta \mapsto \theta_{a,b}(\zeta|\omega) \]
Figure 3. Left: spectrum of $D(\alpha)$ as $\alpha$ varies. Right: level surface of $k \mapsto \| (D(\alpha) - k)^{-1} \| = 10^2$ as $\alpha$ varies: we see that the norm of the resolvent $(D(\alpha) - k)^{-1}$ grows as we approach the first two magic $\alpha$'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.

\[(1) \quad 1/\alpha \in \text{Spec}_{L^2(\mathbb{C}/\Gamma)}(T_k), \quad k \notin \Gamma^*; \]
\[(2) \quad \text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \mathbb{C}; \]
\[(3) \quad 0 \in \bigcap_{k \in \mathbb{C}} \text{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_k(\alpha)), \text{ where } H_k \text{ is defined in (1.3)}. \]

We denote the full set of resonant $\alpha$’s and the set of magic $\alpha$’s as
\[A := 1/(\text{Spec}_{L^2(\mathbb{C}/\Gamma)}(T_k) \setminus \{0\}), \quad k \notin \Gamma^*, \]
\[A_{\text{mag}} := A \cap (0, \infty) = \{\alpha_j\}_{j \geq 1}, \quad \alpha_1 < \alpha_2 < \cdots, \]
respectively. The elements of $A$ are included with their multiplicities as multiplicities of eigenvalues of $T_k$. As a simple byproduct of Theorems 1 and 2 we have
\[\text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \Gamma^*, \quad \alpha \notin A. \]

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

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

**Theorem 3.** For the potential $U$ given by (1.2) we have
\[\sum_{\alpha \in A} \alpha^{-4} = 72\pi/\sqrt{3}, \]
where $\alpha$’s are included according to their multiplicities. In particular, $A \neq \emptyset$. 

Concerning \( A_{\text{mag}} \), an intriguing asymptotic relation for \( \alpha_j \)'s for \( U \) given by (1.2) was suggested by the numerics in [TKV19]:

\[
\alpha_{j+1} - \alpha_j \simeq \frac{3}{2}, \quad j \gg 1.
\]

(1.10)

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 \( \alpha \) 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 \( H_k(\alpha) \) is given by (1.1) and (1.3) with \( U \) given by (1.2) and that

\[
\text{Spec}_{L^2(\mathbb{C}/\Gamma)} H_k(\alpha) = \{ E_j(k, \alpha) \}_{j \in \mathbb{Z}}, \quad E_j(k, \alpha) \leq E_{j+1}(k, \alpha), \quad k \in \mathbb{C}, \quad \alpha > 0,
\]

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

\[
|E_j(k, \alpha)| \leq c_0 e^{-c_1 \alpha}, \quad |j| \leq c_2 \alpha, \quad \alpha > 0.
\]

(1.11)

Numerical experiments presented in Figure 7 (see also Figure 4) suggest that for any \( c_2 \) there exists \( c_0 \) for which (1.11) holds, with \( c_1 = 1 \). The theorem is proved by showing that for large \( \alpha \) 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 $H_k(\alpha)$ is self-adjoint, having a zero eigenvalue is equivalent to $k \in \text{Spec}(D(\alpha))$ 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 (2.1), 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 $U \equiv 0$.)

2. HAMILTONIAN AND ITS SYMMETRIES

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

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

\[ a = \frac{4}{3} \pi i \omega^\ell, \quad \ell \in \mathbb{Z}_3 \implies U(z + a) = \bar{\omega} U(z), \quad U(\omega z) = \omega U(z). \]  

(2.1)

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

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

From this first property in (2.1) we see that

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

(2.2)

The dual lattice consisting of $k$ satisfying \( \frac{1}{2}(\gamma \bar{k} + \bar{\gamma} k) \in 2\pi \mathbb{Z} \) 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 $L_a \mathbf{v}(z) := \mathbf{v}(z + a)$,

\[ D(\alpha)L_a = L_a \begin{pmatrix} 2D_z \\ \bar{\omega} \alpha \bar{U}(-\bullet) \\ 2D_z \end{pmatrix} L_a = \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix} L_a D(\alpha) \begin{pmatrix} \bar{\omega} & 0 \\ 0 & 1 \end{pmatrix}, \quad a = \frac{4}{3} \pi i \omega^\ell, \quad \ell = 1, 2. \]

Hence,

\[ \mathcal{L}_a D(\alpha) = D(\alpha) \mathcal{L}_a, \quad \mathcal{L}_a := \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix} L_a, \quad a = \frac{4}{3} \pi i \omega^\ell, \quad \ell = 1, 2. \]  

(2.3)

Putting

\[ \Gamma_3 := \Gamma / 3 = \frac{4}{3} \pi (i\omega \mathbb{Z} \oplus i\omega^2 \mathbb{Z}), \quad \Gamma_3 / \Gamma \simeq \mathbb{Z}_3^2, \]  

(2.4)

and

\[ \mathcal{L}_a := \begin{pmatrix} \omega^{a_1+a_2} & 0 \\ 0 & 1 \end{pmatrix} L_a, \quad a = \frac{4}{3} \pi i (\omega a_1 + \omega^2 a_2), \]

we obtain a unitary action of $\Gamma_3$ on $L^2(\mathbb{C})$ or on $L^2(\mathbb{C}/\mathbb{C})$, $\Gamma_3 \ni a \mapsto \mathcal{L}_a$.

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

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

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

$$\pi_k : \mathbb{Z}_3^2 \to U(1), \quad \pi_k(a) = e^{\frac{i}{2}(ak + \bar{a}k)},$$

$$e^{\frac{i}{2}(ak + \bar{a}k)}a = \frac{4}{\pi}(a_1i\omega + a_2i\omega^2), \quad a_j \in \mathbb{Z}_3, \quad k = \frac{1}{\sqrt{3}}(\omega^2k_1 - \omega k_2), \quad k_j \in \mathbb{Z}_3,$$

$$\frac{1}{2}(\bar{a}k + ak) = \langle a, k \rangle = \frac{2\pi}{3}(k_1a_1 + k_2a_2).$$

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

$$\rho_{k,p}((a, \ell)) = \tilde{\omega}^{\ell p}\pi(k,k)(a),$$

or three dimensional, for $k \notin \Delta$:

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

The representations are equivalent for $k$ in the same orbit of the transpose of $a \mapsto \omega a$, 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:

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

where the $e_j$ form the standard basis elements of $\mathbb{C}^4$. The action of $G_3 = \mathbb{Z}_3^2 \times \mathbb{Z}_3$ is diagonal and, with $a = \frac{4}{\pi}(a_1i\omega + a_2i\omega^2),$

$$\mathcal{L}_a e_1 = \omega^{a_1+a_2} e_1, \quad \mathcal{L}_a e_2 = e_2, \quad \mathcal{L}_a e_3 = \omega^{a_1+a_2} e_3, \quad \mathcal{L}_a e_4 = e_4,$$

$$\mathcal{C} e_1 = e_1, \quad \mathcal{C} e_2 = e_2, \quad \mathcal{C} e_3 = \omega e_3, \quad \mathcal{C} e_4 = \omega e_4.$$
These observations imply that, with $L^2_{\rho,k,p} := L^2_{\rho,k,p}(\mathbb{C}/\Gamma;\mathbb{C}^4)$,

\[ e_1 \in L^2_{\rho,1,0}, \quad e_2 \in L^2_{\rho,0,0}, \quad e_3 \in L^2_{\rho,1,1}, \quad e_4 \in L^2_{\rho,0,1}. \]

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 $\mathcal{W}$ (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 $H_{k,\ell}(\alpha)$, $k, \ell$ 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 $\alpha \in \mathbb{C}$,

\[ \ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^4)} D(\alpha) \neq \{0\}. \]

In the notation of (1.5), $\ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha) = \mathcal{E} \ker_{L^2(\mathbb{C}/\Gamma;\mathbb{C}^2)} D(\alpha) \neq \{0\}$.

### 2.3. Floquet theory

Since the statement (1.3) 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 $\Gamma$ (see (2.2))

\[ \Gamma \ni a : \psi \mapsto L_a \psi(z) = \psi(z + a), \quad \psi \in L^2(\mathbb{C};\mathbb{C}^2), \quad D(\alpha) L_a = L_a D(\alpha). \]

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

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

\[ \text{Spec } D(0) = \Gamma^*, \quad D(0) e_k e_j = k e_k e_j, \quad e_k(z) := e^{z(kz + k^2)}, \quad k \in \Gamma^*, \quad j = 1, 2, \quad (2.8) \]

where the exponentials $e_k/\text{vol}(\mathbb{C}/\Gamma)^{\frac{1}{2}}$ form an orthonormal basis of $L^2(\mathbb{C}/\Gamma)$ and $e_j$ 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 $\alpha$

\[ \text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) + k, \quad k \in \Gamma^*. \quad (2.9) \]

**Proof.** Since $D_2$ 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 (2.8), $D(0) - k$ is invertible for $k \notin \Gamma^*$ 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 (2.9), note that if $(D(\alpha) - \lambda)u = 0$ then $(D(\alpha) - (\lambda + k))(e_ku) = 0, k \in \Gamma^*$.  

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

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

This means that 

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

satisfies 

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

It follows that 

$$
e^{\frac{i}{2}(z\bar{k} + \bar{z}k)}H(\alpha)e^{\frac{i}{2}(z\bar{k} + \bar{z}k)} = H_k(\alpha) := \begin{pmatrix}
0 & D(\alpha)^* - \bar{k} \\
D(\alpha) - k & 0
\end{pmatrix}, \quad (2.10)
$$

where $H_k(\alpha)$ is the operator in (1.3).

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

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

We then have 

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

that is, for a fixed $k \in \mathbb{C}/\Gamma^*$, $U H U^*$ acts on periodic functions with respect to $\Gamma$ as the operator in (2.10). For each $k$, the operator $H_k(\alpha)$ 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 $L^2(\mathbb{C})$: 

$$
\text{Spec}_{L^2(\mathbb{C})}(H(\alpha)) = \bigcup_{k \in \mathbb{C}/\Gamma^*} \text{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_k(\alpha)), \quad (2.11)
$$

$$
\text{Spec}_{L^2(\mathbb{C}/\Gamma)}(H_k(\alpha)) = \{ \pm E_j(k, \alpha) \}_{j=0}^\infty, \quad E_{j+1}(k, \alpha) \geq E_j(k, \alpha) \geq 0.
$$

To see the last statement we recall that 

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

Hence, the non-zero eigenvalues of $H_k$ are given by $\pm$ the non-zero singular values of $D(\alpha) + k$ (that is, the eigenvalues of $[(D(\alpha) + k)^* (D(\alpha) + k)]^{\frac{1}{2}}$, included according to their multiplicities). We need to check that the eigenvalue 0 of $(D(\alpha) + k)^* (D(\alpha) + k)$ has the same multiplicity as the zero eigenvalue of $(D(\alpha) + k)(D(\alpha) + k)^*$, so that eigenvalues $E_j(k, \alpha) = 0$ are included exactly twice (for $\pm$).
For that we use Proposition 2.3, which also shows that \( D(\alpha) + k \) is a Fredholm operator of order zero, and hence
\[
\dim \ker(D(\alpha) + k) = \dim \ker(D(\alpha)^* + \bar{k}).
\]
In (2.11) we abuse notation by counting ±0 twice in the spectrum of \( H_k(\alpha) \).

From this discussion we can re-interpret (1.3) as the existence of a flat band:

**Proposition 2.4.** In the notation of (1.3) and (2.11)
\[
0 \in \bigcap_{k \in \mathbb{C}} \text{Spec } H_k(\alpha) \iff E_0(k, \alpha) = 0 \text{ for all } k \in \mathbb{C}/\Gamma^*.
\]  

(2.12)

3. Resonant and magic angles

We now want to obtain a computable condition on \( \alpha \) guaranteeing (1.3), that is, the flatness of a band (2.12). In view of (2.10) and (2.11), (1.3) is equivalent to \( \text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \mathbb{C} \).

3.1. Spectrum of \( D(\alpha) \). To investigate the spectrum of \( D(\alpha) \) we use the operator \( T_k \) defined in (1.7). We note that for \( k \notin \Gamma^* \), (2.8) shows that
\[
D(\alpha) - k = (D(0) - k)(I + \alpha T_k), \quad D(0) = 2D_z.
\]  

(3.1)
The operator \( T_k : L^2(\mathbb{C}/\Gamma; \mathbb{C}^2) \rightarrow L^2(\mathbb{C}/\Gamma; \mathbb{C}^2) \) is compact and hence its spectrum can only accumulate at 0. This means that
\[
\Gamma^* \not\ni k \in \text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) \iff \alpha \in \mathcal{A}_k, \quad \mathcal{A}_k := \frac{1}{\text{Spec}(T_k) \setminus \{0\}},
\]  

where \( \mathcal{A}_k \) 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 Theorem 1.

**Proposition 3.1.** For \( k \notin \Gamma^* \), the discrete set \( \mathcal{A} = \mathcal{A}_k \) is independent of \( k \) and
\[
\text{Spec}_{L^2(\mathbb{C}/\Gamma)}(D(\alpha)) = \begin{cases} \Gamma^*, & \alpha \notin \mathcal{A}; \\ \mathbb{C}, & \alpha \in \mathcal{A}. \end{cases}
\]  

(3.3)

Moreover, for all \( \alpha \notin \mathcal{A} \),
\[
\ker_{L^2(\mathbb{C}/\Gamma; \mathbb{C}^2)} D(\alpha) = \mathbb{C}u(\alpha) \oplus \mathbb{C}e^1(\alpha), \quad u(\alpha) \in L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma; \mathbb{C}^2), \quad e^1(0) = e_1.
\]  

(3.4)

where \( \mathcal{E} \) is defined in (1.5) and \( e_1 = (1,0)^t \). For \( \alpha \in \mathbb{R} \), \( u \) extends to a real analytic family, \( \mathbb{R} \ni \alpha \mapsto u(\alpha) \in \ker_{L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma; \mathbb{C}^2)} D(\alpha) \).

**Proof.** Suppose \( \alpha \in \mathbb{C} \setminus \mathcal{A}_k \), \( k \notin \Gamma^* \). Then \( (D(\alpha) - k)^{-1} : L^2(\mathbb{C}/\Gamma) \rightarrow H^1(\mathbb{C}/\Gamma) \hookrightarrow L^2(\mathbb{C}/\Gamma) \) is a compact operator and hence \( D(\alpha) \) has discrete spectrum. By Proposition 2.2, \( 0 \in \text{Spec}(D(\alpha)) \) for all \( \alpha \in \mathbb{C} \), and thus together with the periodicity condition (2.9) this implies \( \text{Spec}(D(\alpha)) \supset \Gamma^* \). Recall now that \( D(\alpha) \) depends on \( \alpha \)
holomorphically and 0 is isolated in the spectrum for \( \alpha \not\in A_k \). Thus, \( \ker_{L^2(\mathbb{C}/\Gamma; \mathbb{C}^2)} D(\alpha) \) depends holomorphically on \( \alpha \not\in A_k \) \([K80, VII. Theorem 1.7]\) 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
\[
\dim(\ker_{L^2(\mathbb{C}/\Gamma; \mathbb{C}^2)} D(\alpha)) = \dim(\ker_{L^2(\mathbb{C}/\Gamma; \mathbb{C}^2)} D(0)) = 2.
\]

The discreteness of the spectrum implies that the spectrum depends continuously on \( \alpha \) \([K80, II. \S6]\) for \( \alpha \not\in A_k \). Since \( \dim(\ker_{L^2(\mathbb{C}/\Gamma; \mathbb{C}^2)} D(\alpha)) = 2 \) for all \( \alpha \not\in A_k \) and by periodicity (2.9), this implies that \( \text{Spec}(D(\alpha)) = \Gamma^* \).

Using (3.2) and that \( \text{Spec}(D(\alpha)) = \Gamma^* \) for all \( \alpha \not\in A_k \), it follows that
\[
\exists k \not\in \Gamma^* \text{ such that } \alpha \not\in A_k \implies \forall p \not\in \Gamma^* \text{ we have } \alpha \not\in A_p.
\]
This shows independence of \( A_k =: A \) of \( k \).

Since
\[
\mathbb{C} \ni \alpha \mapsto \tilde{H}(\alpha) := \begin{pmatrix} 0 & D(\bar{\alpha})^* \\ D(\alpha) & 0 \end{pmatrix}, \quad \tilde{H}(\alpha) = H(\alpha), \quad \alpha \in \mathbb{R},
\]
is a holomorphic operator family with compact resolvents, self-adjoint for \( \alpha \in \mathbb{R} \), Rellich’s theorem \([K80, VII. Theorem 3.9]\) implies that all eigenvalues and eigenfunctions of \( H(\alpha) = \tilde{H}(\alpha) \) are real-analytic for \( \alpha \in \mathbb{R} \). If we let \( \varphi(\alpha) := (u(\alpha), 0, 0)^t \in L^2_{\rho_1, \rho}, \alpha \in \mathbb{R} \setminus A, \) then \( \varphi(0) = e_1 \in \mathbb{C}^4 \) and by the discussion above \( \varphi(\alpha) \) extends to a real analytic family for all \( \alpha \in \mathbb{R} \).

The next proposition provides the symmetries of the set \( A \).

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

**Proof.** To see the symmetries of the spectrum, we note that since \( Qv(z) = \overline{v(-\bar{z})} \), the anti-linear involution satisfies
\[
D(\alpha)Qv = -QD(-\alpha)^*v,
\]
which in turn implies \( \text{Spec } D(\alpha) = -\text{Spec } D(-\alpha)^* = -\text{Spec } D(-\alpha) \). But then (3.3) shows that \( \text{Spec } D(\alpha) = \text{Spec } D(-\alpha) \).

Next we notice that \( \overline{U(\bar{z})} = U(z) \). If we define the unitary map \( Fv(z) := \overline{v(\bar{z})} \), then we find using \( (DzFv)(z) = (Dz\overline{v})(\bar{z}) = -(\overline{Dzv})(\bar{z}) = -(FDzv)(z) \) the relation
\[
D(\alpha)(Fv) = -F(D(-\bar{\alpha})v),
\]
which implies that \( \text{Spec}(D(\alpha)) = -\text{Spec}(D(-\bar{\alpha})) = \text{Spec}(D(\bar{\alpha})) \). In these statements \( \text{Spec} \) can be either the spectrum on \( L^2(\mathbb{C}), \text{Spec}_{L^2(\mathbb{C})} \), or on \( L^2(\mathbb{C}/\Gamma), \text{Spec}_{L^2(\mathbb{C}/\Gamma)} \). □
The description of the kernel of $D(\alpha)$ gives us an expression for the inverse of $D(\alpha) - k$, $k \notin \Gamma^*$ and $\alpha \notin \mathcal{A}$. We start with the following simple

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

$$V(\alpha) := [u(\alpha), \mathcal{S}u(\alpha)], \quad v(\alpha) := \det V(\alpha).$$

Then $v(\alpha) \neq 0$ and $k \notin \Gamma^*$ imply that

$$(D(\alpha) - k)^{-1} = \frac{1}{v(\alpha)} \operatorname{adj}(V(\alpha))(2D_z - k)^{-1}(V(\alpha)). \quad (3.5)$$

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

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

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

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

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 $\theta$ functions – see [Mu83]. We have

$$\theta_{a,b}(z|\tau) := \sum_{n \in \mathbb{Z}} \exp(\pi i (a + n)^2 \tau + 2\pi i (n + a)(z + b)), \quad \operatorname{Im} \tau > 0,$$

$$\theta_{a,b}(z + 1|\tau) = e^{2\pi ia} \theta_{a,b}(z|\tau), \quad \theta_{a,b}(z + \tau|\tau) = e^{-2\pi i(z+b) - \pi i\tau} \theta_{a,b}(z|\tau), \quad (3.6)$$

$$\theta_{a+1,b}(z|\tau) = \theta_{a,b}(z|\tau), \quad \theta_{a,b+1}(z|\tau) = e^{2\pi ia} \theta_{a,b}(z|\tau).$$

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

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

If

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

then (3.6) shows that

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

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

With this in place we can prove
Figure 5. Plots of $z \mapsto \log |u(\alpha, z)|$ (in the notation of Proposition 3.1) for $\alpha$ 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 $u$ at $z_S = \frac{4\sqrt{3}}{9}\pi$ is close to 0.
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 \( u(\alpha) = (\psi_1, \psi_2) \) then
\[ v(\alpha) = \psi_1(z)\psi_1(-z) + \psi_2(z)\psi_2(-z). \]
As remarked after (1.4), \( v(\alpha) \) is independent of \( z \).

The observation made in [TKV19] is that \( \psi_2 \) vanishes at special stacking points. These are fixed points of the action \( z \mapsto \omega z \) on \( \mathbb{C}/\Gamma_3 \) (see (2.4)):
\[ \psi_2(\alpha, \pm z_S) = 0, \quad z_S := \frac{1}{3}(a_2 - a_1) = \frac{4\pi j}{3}, \quad a_j = \frac{2}{3}\pi i\omega^j. \tag{3.10} \]
To see this, note that (with the action of \( \mathcal{C} \) identified with the action on \( (u, 0z^t)^t \in L^2(\mathbb{C}/\Gamma; \mathbb{C}^4) \))
\[ u(\alpha, \pm z_S) = (\mathcal{C}u)(\alpha, \pm \omega z_S) = u(\alpha, \pm z_S \mp a_2) = (\begin{pmatrix} \omega^{\pm 1} & 0 \\ 0 & 1 \end{pmatrix} \mathcal{L}_{a_2}u)(\alpha, \pm z_S) = (\begin{pmatrix} 1 & 0 \\ 0 & \omega^{\mp 1} \end{pmatrix}) u(\alpha, \pm z_S). \]
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 \( u(\alpha, z_S) = 0 \) or \( u(\alpha, -z_S) = 0 \). Assume the former holds (otherwise we replace \( u \) with \( \mathcal{C}u \)). We can then construct a periodic solution to \( (D(\alpha) - k)v_k = 0 \) for any \( k \in \mathbb{C} \), and in particular for \( k \notin \Gamma^* \), implying, in view of (3.3), that \( \alpha \in \mathcal{A} \).

In fact, if \( f_k \) is holomorphic with simple poles at the zeros of \( u \) allowed (we note that the equations \( 2D_z\psi_1 + U(z)\psi_2 = 2D_z\psi_2 + U(-z)\psi_1 = 0 \) imply that \( \partial_z^j\psi_j(z_S) = 0 \) and hence \( u = (z - z_S)\tilde{u} \), where \( \tilde{u} \) is smooth near \( z_S \) then
\[ (D(\alpha) - k)v_k = 0, \quad v_k(z) = e^{\frac{i}{2}(z\ell + zk)}f_k(z)v(z). \]
To obtain periodicity we need
\[ f_k(z + a) = e^{-\frac{i}{2}(ak + a^2)}f_k(z), \quad a \in \Gamma, \quad \frac{1}{2}(a\tilde{k} + \tilde{a}k) = 2\pi(a_1k_1 + a_2k_2), \]
\[ a = 4\pi(a_1\omega + a_2\omega^2), \quad k = \frac{1}{\sqrt{3}}(k_1\omega^2 - k_2\omega). \]
But now, (3.7)–(3.9) show that we can take
\[ f_k(z) = \frac{\theta_{-\frac{1}{2}+k_1/3,\frac{1}{2}-k_2/3}(3z/4\pi i\omega)|\omega)}{\theta_{-\frac{1}{2}+k_1/3,\frac{1}{2}-k_2/3}(3z/4\pi i\omega)|\omega}. \]

Proof of Theorem 2. The lack of dependence of the spectrum of \( T_k \) on \( k \notin \Gamma^* \) and equivalence of statements (1) and (2) are the content of Proposition 3.1. The definition of \( H_k(\alpha) \) in (1.3) immediately shows their equivalence to statement (3). \( \square \)
Proof of Theorem 1. In Proposition 3.1 we already obtained a (real) analytic family \( \alpha \mapsto u(\alpha) \). Then \( v(\alpha) = W(u(\alpha), \delta' u(\alpha)) \) and the equivalence of \( v(\alpha) \) to (1) in Theorem 2 follows from Proposition 3.3 and 3.4. □

Remarks. 1. The zero of \( u(\alpha) \in \ker L^2 \oplus \mathbb{C}/\Gamma \) \( D(\alpha) \) 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 \( \delta' u(z) = f(z) u(z) \), where, using \( v(\alpha) = 0 \) again, \[
\frac{f(z) := \psi_2(-z)}{\psi_1(z)} = \frac{-\psi_1(-z)}{\psi_2(z)} = \frac{aU(z)\psi_1(-z)}{2D_2\psi(z)} ,
\]
(3.11) is holomorphic away from \( \psi_1^{-1}(0) \cap (D_2\psi_1)^{-1}(0) \). 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 \( F_j : B_{C^2}(0, \delta) \to \mathbb{C} \) are holomorphic functions (this follows from real analyticity of \( \psi_j \), which follows in turn from the ellipticity of the equation – see [HöI, Theorem 8.6.1]). The definition of \( f \) and the fact that \( \partial_2 f = 0 \) away from zeros of \( \psi_1 \) shows that \( F_2(\zeta, \bar{\zeta}) = f(z_0 + \zeta)F_1(\zeta, \bar{\zeta}) \). We can then choose \( \xi_0 \) such that \( F_1(\zeta, \bar{\zeta}) \) is not identically zero (if no such \( \xi_0 \) existed, \( \psi_1 \equiv 0 \), and hence, from the equation, \( u \equiv 0 \)). But then \( \zeta \mapsto f(z_0 + \zeta) = F_2(z_0, \xi_0)/F_1(z_0, \xi_0) \) is meromorphic near \( \zeta = 0 \) and, as \( z_0 \) was arbitrary, everywhere. In addition, \[
f(z + a) = \omega^{-a_1-a_2} f(z), \quad a \in \Gamma_3, \quad f(\omega z) = f(z), \quad f(z) f(-z) = -1 .
\]
These symmetries also show that \( f(z_S + \omega \zeta) = \omega^{-1} f(z_S + \zeta) \), which means that \( f(z_S + \zeta) = \sum_{k \geq k_0} \zeta^{-1+3k} \zeta \) and \( f(-z_S - \zeta) = \sum_{\ell \geq -k_0} \zeta^{-2+3\ell} \zeta \), for some \( k_0 \in \mathbb{Z} \). Hence, if \( f \) has only poles of order 1, we have \( u(\alpha, z_S) = 0 \). We formulate this bold guess as follows: \[
u(\alpha) \in \ker L^2 \oplus \mathbb{C}/\Gamma \) \( D(\alpha) \), \( u(\alpha) \neq 0 \implies u(\alpha, z) \neq 0 , \quad z \notin z_S + \Gamma_3 \) \( (3.12) \)
\]
This is related to the following fact, which seems to hold as well: \[
\dim \ker L^2 \oplus (\mathbb{C}/\Gamma \) \( D(\alpha) = 1 \) , \( \alpha \in \mathbb{C} \) \( (3.13) \)
\]
Proof of (3.12) \( \implies \) (3.13). Suppose that \( u = (\psi_1, \psi_2)^t \) and \( v = (\varphi_1, \varphi_2)^t \) are two elements of the kernel in \( L^2 \oplus \mathbb{C}/\Gamma \). 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 \( v = gw \), 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 \( \Gamma_3 \). From (3.12) applied to \( \psi_1 \) we see that \( g \) can only have poles at \( z_S \) and, applied to \( \varphi_1(z) \) see that \( g \) can only have zeros at the same place. But this implies that \( g \) is constant. □

2. The elements of the kernel of \( D(\alpha) - k \) 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 \((2D_2 - k)^{-1} \) 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 $2D_z - k$ on $\mathbb{C}/\Gamma$. To obtain the convolution kernel (in a construction which works for any torus) we seek a function $G_k$ such that

$$(2D_z - k)G_k = \delta_0(z), \quad G_k = e^{\frac{k}{2}(z^2 + k^2)}g_k(z), \quad \partial_z g_k|_{\gamma = \Gamma} = 0,$$

$$g_k(z + a) = e^{-\frac{1}{2}(ka + k\bar{a})}g_k(z), \quad \text{Res}_{z = w}g_k(z) = \begin{cases} i/(2\pi), & w \in \Gamma; \\ 0, & w \notin \Gamma. \end{cases}$$

(The last condition gives $2D_z g_k(z) = \sum_{\alpha \in \Gamma} \delta_{\alpha}(z)$, as $\partial_z (1/(\pi z)) = \delta_0(z)$.)

To find $g_k$ we return to (3.7) and (3.8) and choose

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

Hence we have

$$g_k(z) := \frac{e^{-\pi i k_1^2 + \pi i k_1(\frac{1}{2} + k_2)^2} \theta_{\frac{1}{2}}^\omega(0|\omega) \theta_{\frac{1}{2}}^{\frac{1}{2} - k_1 + \frac{1}{2} + k_2}(z/4\pi i\omega|\omega)}{2\pi i \theta_{\frac{1}{2}}^\omega(\omega k_1 + k_2)|\omega \theta_{\frac{1}{2}}^{\frac{1}{2} - k_1 + \frac{1}{2} + k_2}(z/4\pi i\omega|\omega)}, \quad (k_1, k_2) \notin \mathbb{Z}^2. \tag{3.14}$$

It would be interesting to derive (1.6) from (3.5) and (3.14). \hfill \square

3.3. **Existence of magic $\alpha$’s.** We now give a proof of Theorem 3 which amounts to calculating $\text{tr} T_k^4$. 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 $2D_z = D_{x_1} + iD_{x_2} = (\omega^2 D_{y_1} - \omega D_{y_2})/\sqrt{3}$. We are then studying

$$D_k(\alpha) := D(\alpha) + k = \frac{1}{\sqrt{3}} \left( \begin{array}{cc} \mathcal{D}_k & \alpha \mathcal{V}(y) \\ \mathcal{V}(-y) & \mathcal{D}_k \end{array} \right), \quad \mathcal{V}(y) := \sqrt{3}(e^{-i(y_1 + y_2)} + \omega e^{i(2y_1 - y_2)} + \omega^2 e^{i(-y_1 + 2y_2)}),$$

with periodic boundary conditions (for $y \mapsto y + 2\pi n$, $n \in \mathbb{Z}^2$). The operator $T_k, k = (\omega^2 k_1 - \omega k_2)/\sqrt{3}, (k_1, k_2) \notin \mathbb{Z}^2$, is given by

$$T_k := \left( \begin{array}{cc} 0 & \mathcal{V}_+ \\ \mathcal{D}_k^{-1} \mathcal{V}_- & 0 \end{array} \right).$$

In this notation,

$$\text{tr} T_k^4 = 18 \text{tr} A^2, \quad A := A_k := \frac{1}{3} \mathcal{D}_k^{-1} \mathcal{V}_+ \mathcal{D}_k^{-1} \mathcal{V}_-, \tag{3.16}$$

where we note that $A^2$, a pseudodifferential operator of order $-4$, is of trace class (see for instance [DyZw19, Theorem B.21]).
Proof. We notice that (this can be checked by taking a common denominator using
where the first term on the right hand side vanishes and both series converge absolutely

\[ \sum \]

Using the partial fraction expansion, the fact that \( \wp \) for the

Also, if we define\( F \) then

For \( \Gamma := \omega \mathbb{Z} \oplus \mathbb{Z}, \omega := e^{2\pi i/3} \) and \( \gamma_0 \in \Gamma \setminus \{0\} \) define

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

Then

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

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

\[ g(\gamma_0) := \sum_{j=0}^{2} \omega^j K(\omega^j \gamma_0) = 3K(\gamma_0). \] (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 \( \Gamma \)-periodic function with the singularity at \( z = 0 \) given by \( 2/(z\gamma_0)^2 \). Hence,

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

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

\[
\begin{align*}
 g(\gamma_0) &= \sum_{j=0}^{2} \omega^j F(z, \omega^j \gamma_0) = \gamma_0^{-2} \sum_{\gamma \in \Gamma} \sum_{j=0}^{2} \tilde{\omega}^j \left( \frac{1}{(\gamma - \omega^j \gamma_0 - z)^2} - \frac{2\tilde{\omega}^j}{\gamma_0} \frac{1}{(\gamma - \omega^j \gamma_0 - z)} \right) \\
 &= \gamma_0^{-2} \sum_{j=0}^{2} \tilde{\omega}^j \varphi(z) + \sum_{\gamma \in \Gamma} \sum_{j=0}^{2} \tilde{\omega}^j \frac{1 - \delta_{\gamma,0}}{\gamma_0} \frac{1}{(\gamma - \omega^j \gamma_0 - z)^2} - \sum_{\gamma \in \Gamma} \sum_{j=0}^{2} \omega^j \frac{1}{\gamma_0^3} \frac{1}{(\gamma - \omega^j \gamma_0 - z)},
\end{align*}
\]

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
\[
\sum_{\gamma} \sum_{j=0}^{2} \frac{\omega^j}{(\gamma - \omega^j \gamma_0)^2} = \lim_{N \to \infty} \sum_{j=0}^{2} \omega^j \sum_{|\gamma - \omega^j \gamma_0| \leq N} (1 - \delta_{\gamma,0}) \gamma^{-2} = \mathcal{O}(1) \lim_{N \to \infty} \sum_{N-|\gamma| \leq |\gamma|} N^{-2} = 0.
\]
Hence, using the fact that \(\sum_{n \in \mathbb{Z}}((n-a)^{-1} - (n-b)^{-1}) = \pi \cot \pi b - \pi \cot \pi a\),
\[
g(\gamma_0) = 2\pi \gamma_0^{-3} \lim_{M \to \infty} \sum_{m=-M}^{M} \sum_{j=0}^{2} \omega^j (\cot \pi (m\omega + \omega^j \gamma_0 + z) - \cot \pi (m\omega + z)), \quad (3.21)
\]
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 \(a_m := (e^{2\pi i (m\omega + z)} - 1)^{-1}\),
\[
\sum_{m=-M}^{M} (\cot((m + m_0)\omega + n_0 - z) - \cot \pi (m\omega + z)) = 2i \sum_{m=-M}^{M+m_0} (a_{m+m_0} - a_m) = 2i \sum_{m=M+1}^{M+m_0} a_m - 2i \sum_{m=-M}^{M} a_m = 2i \sum_{m=M+1}^{M+m_0} (-1 + \mathcal{O}(e^{-M})) - 2i \sum_{m=M-m_0+1}^{M} \mathcal{O}(e^{-M}) = -2im_0 + \mathcal{O}(e^{-M}).
\]
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:
\[
J^{p,q} := J^p \otimes J^q, \quad p, q \in \mathbb{Z}. \quad (3.22)
\]
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:
\[
\Lambda_{p,q} := (\Lambda_{i+p,j+q})_{i,j \in \mathbb{Z}}, \quad (\Lambda \Lambda')_{p,q} = \Lambda_{p,q} \Lambda'_{p,q}, \quad (\Lambda_{p',q'})_{p,q} = \Lambda_{p+p',q+q'}, \quad (3.23)
\]
where \(\Lambda'\) is just another diagonal matrix. To express powers of \(A\) in (3.16) we will use the following simple fact:
\[
J^{p,q} \Lambda J^{p',q'} = \Lambda_{p,q} J^{p+p',q+q'} = J^{p+p',q+q'} \Lambda_{-p'-q',-q'}. \quad (3.24)
\]
If we put
\[ \Lambda := D_k^{-1}, \quad \Lambda_{mn} = (\omega^2 (m + k_1) - \omega (n + k_2))^{-1}, \quad (k_1, k_2) \notin \mathbb{Z}^2, \]
then, in the notation of (3.16),
\[ A = \Lambda (J^{1,1} + \omega J^{-2,1} + \omega^2 J^{1,-2}) \Lambda (J^{-1,-1} + \omega J^{2,-1} + \omega^2 J^{-1,2}) \]
\[ + \omega \Lambda \Lambda_{1,-2} + \omega^2 \Lambda \Lambda_{-2,1} + \omega \Lambda \Lambda_{1,1} J^{3,0} + \omega^2 \Lambda \Lambda_{1,1} J^{0,3} \]
\[ + \omega \Lambda \Lambda_{-2,1} J^{-3,0} + \omega^2 \Lambda \Lambda_{-2,1} J^{0,-3} + \Lambda_{1,-2} J^{-3,3} + \Lambda_{1,-2} J^{3,-3}. \]

The diagonal part of \( A^2 \) is then given by (note that the matrices are diagonal and commute)
\[ B := \Lambda^2 \Lambda_{1,1} + \omega^2 \Lambda^2 \Lambda_{1,-2} + \omega \Lambda^2 \Lambda_{1,1} \Lambda_{1,-2} + 2 \omega^2 \Lambda^2 \Lambda_{1,1} \Lambda_{-2,1} \]
\[ + 2 \Lambda^2 \Lambda_{-2,1} \Lambda_{1,-2} + \omega^2 \Lambda^2 \Lambda_{-2,1} \Lambda_{3,0} + \omega^2 \Lambda^2 \Lambda_{-2,1} \Lambda_{3,-3} + \omega \Lambda^2 \Lambda_{1,1} \Lambda_{0,3} \]
\[ + \omega \Lambda^2 \Lambda_{-2,1} \Lambda_{0,-3} + \Lambda^2 \Lambda_{-2,1} \Lambda_{-3,3} + \Lambda^2 \Lambda_{-2,1} \Lambda_{-3,-3}. \]

Since \( \text{tr} \Lambda_{k,l}^2 \Lambda_{p,q} \Lambda_{p',q'} = \text{tr} \Lambda_{k,r+s}^2 \Lambda_{p+r,q+s} \Lambda_{p'+r,q'+s} \), we have
\[ \text{tr} A^2 = 2 \Lambda^2 (\Lambda_{1,1} + 2 \Lambda_{2,1} \Lambda_{1,-2} + 2 \Lambda_{2,-1} \Lambda_{-1,2}) \]
\[ + \omega \text{tr} (\Lambda^2 \Lambda_{-2,1} \Lambda_{1,-2} + 2 \Lambda_{1,1} \Lambda_{-2,1} + 2 \Lambda_{1,-2} \Lambda_{-1,1} - \Lambda_{-1,-2} \Lambda_{1,1}) \]
\[ + \omega^2 \text{tr} (\Lambda^2 \Lambda_{1,1} + 2 \Lambda_{1,1} \Lambda_{-2,1} + 2 \Lambda_{-1,1} \Lambda_{2,-1}). \]

We now find that
\[ \Lambda_{\pm 2, \mp 1} \Lambda_{\pm 1, \pm 2} + \omega \Lambda_{\mp 1, \pm 2} \Lambda_{\mp 1, \pm 1} + \omega^2 \Lambda_{\pm 1, \mp 1} \Lambda_{\pm 2, \pm 1} = 0. \]

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 \( n \in \mathbb{Z}^2 \)
\[ \omega (\Lambda_{2,-1})_{n,n}^{-1} + \bar{\omega} (\Lambda_{-1,2})_{n,n}^{-1} + (\Lambda_{-1,-2})_{n,n}^{-1} = 0 \]
which follows from a direct computation. Hence, the expression for the trace simplifies further to
\[ \text{tr} A^2 = \text{tr} \Lambda^2 (\Lambda_{1,1}^2 + \omega \Lambda_{-2,1}^2 + \omega^2 \Lambda_{1,-2}^2), \quad (3.26) \]
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 \( \omega^2 (m + p) - \omega (n + q) = \omega (\gamma - \gamma_0), \gamma_0 = -\omega p + q, \)
\[ \text{tr} A^2 = \bar{\omega} K(-\omega + 1) + K(2\omega + 1) + \omega K(-\omega - 2) \]
\[ = K(2\omega + 1) + \omega K(\omega(2\omega + 1)) + \omega^2 K(\omega^2(2\omega + 1)) = 3K(2\omega + 1) \]
\[ = 4\pi/\sqrt{3}, \]
where we used (3.19) and (3.20). In view of (3.16), this concludes the proof. □

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

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

(4.1)

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

\[
  f_n(z + a) = \bar{\omega}^n f_n(z), \quad a = \frac{4}{3} \pi i \omega^\ell, \quad \ell \in \mathbb{Z}_3.
\]

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

\[
  U(z) = U(z, \bar{z}) = \sum_{n \in \mathbb{Z}^3 + 1} a_n f_n(z, \bar{z}), \quad |a_n| \leq c_0 e^{-c_1|n|},
\]

(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 [GW19] and [WG19], 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 \( U_\mu \) appearing in Figure 2 is obtained by taking \( a_1 = 1, a_{-2} = \mu \) and \( a_n = 0 \) for \( n \neq 1, -2 \).

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

We now impose a generic non-degeneracy assumption that

\[
  \sum_{n \in \mathbb{Z}^3 + 1} n \text{Re}(a_n) \neq 0.
\]

(4.3)

This is trivially satisfied by the standard potential in (1.2), and for the potential \( U_\mu \) 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 \( H_k(\alpha) \) is given by (1.1) and (1.3) with \( U \) given by (4.2) and that

\[
  \text{Spec}_{L^2(\mathbb{C}/\Gamma)} H_k(\alpha) = \{ E_j(k, \alpha) \}_{j \in \mathbb{Z}}, \quad E_j(k, \alpha) \leq E_{j+1}(k, \alpha), \quad k \in \mathbb{C}, \ \alpha > 0,
\]
with the convention that $E_0(k, \alpha) = \min_j |E_j(k, \alpha)|$. If $U$ satisfies (4.3), then there exist positive constants $c_0$, $c_1$, and $c_2$ such that for all $k \in \mathbb{C}$,

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

Remark. If in (4.2) we assumed instead that $|a_n| \leq C_N |n|^{-N}$ for all $N$, that is, that the potential is smooth, then the conclusion would be replaced by $|E_j(k, \alpha)| \leq C_N \alpha^{-N}$ 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

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

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

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

(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

$$\{a, b\} = \sum_{j=1}^2 \partial_{\xi_j}a \partial_{x_j}b - \partial_{\xi_j}b \partial_{x_j}a = \partial_{\zeta}a \partial_{\bar{\zeta}}b - \partial_{\zeta}b \partial_{\bar{\zeta}}a + \partial_\zeta a \partial_{\bar{\zeta}}b - \partial_\zeta b \partial_{\bar{\zeta}}a. \quad (4.5)$$

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 $Q = \sum_{|\alpha| \leq m} a_\alpha(x, h)(hD)^\alpha$ 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

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

then there exists a family $\psi_h \in C^\infty_c(\Omega), \ \Omega$ a neighbourhood of $x_0$, such that

$$|(h\partial_\alpha)^\alpha x Qv_h(x)| \leq C_\alpha e^{-c|h/\alpha|}, \quad \|v_h\|_{L^2} = 1, \quad |(h\partial_\xi)^\alpha v_h(x)| \leq C_\alpha e^{-c|x-x_0|^2/h}, \quad (4.7)$$

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 $k \in \mathbb{C}$ and $z_0 \in \Omega$ there exists a family $h \mapsto u_h \in C^\infty(\mathbb{C}/\Gamma; \mathbb{C}^2)$ such that for $0 < h < h_0$,

$$|(P(h) - h\mathbf{k})u_h(z)| \leq e^{-c|h/\alpha|}, \quad \|u_h\|_{L^2} = 1, \quad |u_h(z)| \leq e^{-c|x-z_0|^2/h}. \quad (4.8)$$
Figure 6. A contour plot of $|\{q, \bar{q}\}| = |\text{Im}(\nabla^\frac{1}{2} \partial_z V)|$ – 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 $V^\frac{1}{2}$.

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 $u_h$ follows from the existence of $v_h \in C^\infty_c(\Omega'; \mathbb{C})$, $\Omega'$ a small neighbourhood of $z_0$ on which $U(z, \bar{z}) \neq 0$, such that

\[
Q v_h = \mathcal{O}(e^{-c/h}) , \quad v_h(z_0) = 1 , \quad |v_h(z)| \leq e^{-c|z-z_0|^2/h} ,
\]

\[
Q := U(z, \bar{z})(2hD_z - h\mathbf{k})(U(z, \bar{z})^{-1}(2hD_z - h\mathbf{k})) - U(-z, -\bar{z})U(z, \bar{z}),
\]

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

\[
u_h := (v_h, -U(z, \bar{z})^{-1}(2hD_z - h\mathbf{k})v_h)
\]

and normalize to have $\|u_h\|_{L^2} = 1$. 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 $2hD_z - h\mathbf{k}$ is $2\zeta$, 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

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

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 $\zeta$ such that

\[
q(z, \bar{z}, \zeta) = 0 , \quad \{q, \bar{q}\}(z, \zeta) \neq 0.
\]
Since \( q = 4\zeta^2 - V(z, \bar{z}) \), we can take \( \zeta = \frac{1}{2} V^{\frac{1}{2}} \) (for either branch of the square root) so that, using (4.5),
\[
i\{q, \bar{q}\} = i(8\zeta \partial_{\zeta} + \partial_z V \partial_{\zeta})(4\zeta^2 - \bar{V}) = 8i(\zeta \partial_{\zeta} V - \bar{\zeta} \partial_{\zeta} \bar{V}) \tag{4.9}
\]
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 \( \text{Im}(V^{\frac{1}{2}} \partial_z V) \) 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
\[
\partial_z f_n(0) = \frac{n}{2} \sum_{k=0}^{2} e^{\frac{n}{2}(z \omega^k - \bar{z} \omega^k)} \bigg|_{z=0} = \frac{3n}{2}, \quad \partial_{\bar{z}} f_n(0) = -\frac{n}{2} \sum_{k=0}^{2} \omega^{2k} e^{\frac{n}{2}(z \omega^k - \bar{z} \omega^k)} \bigg|_{z=0} = 0,
\]
since \( \omega^4 = \omega \) and \( 1 + \omega + \omega^2 = 0 \). Hence,
\[
U(z, \bar{z}) = \partial_z U(0) z + O(|z|^2), \quad \partial_{\bar{z}} U(0) = \frac{3}{2} \sum_{n=3Z+1} na_n. \tag{4.10}
\]
Recall that \( V(z) = U(z) U(-z) \). Since \( U(0) = \partial_z U(0) = 0 \), we have \( V(0) = \partial_z V(0) = \partial_{\bar{z}} V(0) = 0 \), and
\[
\partial_z^2 V(0) = -2(\partial_z U(0))^2, \quad \partial_{\bar{z}} \partial_z V(0) = \partial_{\bar{z}}^2 V(0) = 0.
\]
It follows that
\[
V(z) = -z^2 (\partial_z U(0))^2 (1 + O(|z|)), \quad \partial_z V(z) = -2z (\partial_z U(0))^2 (1 + O(|z|)),
\]
which gives
\[
V^{\frac{1}{2}}(z) \partial_z V(z) = \sqrt{-z^2 (\partial_z U(0))^2 (1 + O(|z|))} \tag{4.3}
\]
From this we see that \( \text{Im}(V^{\frac{1}{2}} \partial_z V) \neq 0 \) in a punctured neighbourhood of the origin if \( \text{Re} \partial_z U(0) \neq 0 \), 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 \( L^2(\mathbb{C}/\Gamma) \).

We can now give
Proof of Theorem 5. In the notation of Proposition 4.1, let $C = [a, b] \times [c, d] \in \Omega$ and consider the finite set $\mathcal{Z}_h := K \sqrt{\hbar} \mathbb{Z}^2 \cap C, \ |\mathcal{Z}_h| \sim 1/h$. Then (4.8) gives $u_n^w, w \in \mathcal{Z}_h$ (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)

$$|\langle u_n^w, u_n^{w'} \rangle| \leq e^{-M|n-n'|^2}, \ n := \frac{w}{K\sqrt{\hbar}}, \ n' := \frac{w'}{K\sqrt{\hbar}} \in \mathbb{Z}^2, \ |u_n^w|_{L^2} = 1. \quad (4.11)$$

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

$$\|H_k(\alpha)u_n^w\|_{L^2(\mathbb{C}/\Gamma)} \leq e^{-c'/h}, \ h = 1/\alpha. \quad (4.12)$$

Using self-adjointness of $H_k$ and in the notation of Theorem 5, write

$$H_k(\alpha)v = \sum_{j \in \mathbb{Z}} E_j(k, \alpha)g_j\langle v, g_j \rangle, \ H_k(\alpha)g_j = E_j(k, \alpha)g_j, \ \langle g_j, g_i \rangle = \delta_{ij}. \quad (4.11)$$

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

$$\dim \text{span}\{g_j\}_{|E_j(k, \alpha)| \geq e^{-c'/2h}} \geq \dim \text{span}\{u_n^w\}_{w \in \mathcal{Z}_h}.$$ 

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

Remark. This simple argument showing exponential squeezing of bands does not apply to the more realistic Bistritzer–MacDonald model of twisted bilayer graphene [BM11]. 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)), $\lambda$, are simple, the Poisson bracket $\{\lambda, \bar{\lambda}\}_{\lambda=0}$ vanishes [B*20].

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

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

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

The discretization is given using a Fourier spectral method; see [Tr00, Chapter 3]. Using the tensor structure of $\mathcal{Z}_k$ and $\mathcal{V}$ we start with the standard orthonormal basis of $L^2(\mathbb{R}^2/2\pi \mathbb{Z}^2)$: $e_n(y) := e_{n_1} \otimes e_{n_2}(y) := e_{n_1}(y_1)e_{n_2}(y_2), e_\ell(t) := (2\pi)^{-\frac{1}{2}} e^{i\ell t}$. Using the
identification \([-N, N] \cap \mathbb{Z} \simeq \mathbb{Z}_{2N+1}\), we define
\[
\Pi_N : L^2(\mathbb{R}^2/2\pi \mathbb{Z}^2; \mathbb{C}^2) \to L^2(\mathbb{Z}_{2N+1}^2; \mathbb{C}^2) = L^2(\mathbb{Z}_{2N+1}; \mathbb{C}^2) \otimes L^2(\mathbb{Z}_{2N+1}; \mathbb{C}^2),
\]
\[
\Pi_N \left( \sum_{n \in \mathbb{Z}^2} a_n e^{i(y,n)} \right) = \{a_{(n_1, n_2)}|_{|n| \leq N}, \quad a_n \in \mathbb{C}^2, \quad n = (n_1, n_2) \in \mathbb{Z}^2,
\]
and \(D^N_k(\alpha) := \Pi_N D_k(\alpha) \Pi_N^*\). Hence,
\[
D^N_k(\alpha) = \frac{1}{\sqrt{3}} \begin{pmatrix} \mathcal{D}^N_k & \alpha \mathcal{Y}^N_+ \\ \alpha \mathcal{Y}^N_- & \mathcal{D}^N_k \end{pmatrix},
\]
where (with \(D^N := \text{diag} (\ell)_{-N \leq |\ell| \leq N}\) and \(J_N\) the \(2N + 1\) dimensional Jordan block)
\[
\mathcal{D}^N_k := \omega^2(D^N + k_1 I_{C_{2N+1}}) \otimes I_{C_{2N+1}} - \omega I_{C_{2N+1}} \otimes (D^N + k_2 I_{C_{2N+1}}),
\]
\[
\mathcal{Y}^N_+ := \sqrt{3}(J_N \otimes J_N + \omega (J_N^k)^t \otimes J_N + \omega^2 J_N \otimes (J_N^k)^t),
\]
\[
\mathcal{Y}^N_- := \sqrt{3}((J_N)^t \otimes (J_N)^t + \omega J_N^k \otimes (J_N)^t + \omega^2 (J_N)^t \otimes J_N^k).\]

The matrix \(D^N_k(\alpha)\) has dimension \(2(2N + 1)^2\). To obtain reasonable accuracy up through the second magic \(\alpha\), 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 \(D^N_k(\alpha)\). To compute the smallest singular values of \(D^N_k(\alpha)\), we use Krylov subspace methods, either the inverse Lanczos algorithm adapted from \([Tr99, Wr02]\) or the augmented implicitly restarted Lanczos method \([BR05]\) implemented in MATLAB’s \texttt{svds} command.

Figure 7 shows numerical calculations of the first 41 non-negative eigenvalues of \(H_k(\alpha)\). As required by Theorem 4, these eigenvalues decay exponentially, apparently no slower than \(e^{-\alpha}\). The vertical lines in the figure indicate the magic \(\alpha\) values. We pursue two approaches to locating these magic \(\alpha \in \mathcal{A}_{\text{mag}}\) (see (1.8) and Theorem 2). The spectral characterization of the set \(\mathcal{A}\) of resonant \(\alpha\)’s via the operator \(T_k\) enables the precise calculation of many points in \(\mathcal{A}\) as reciprocals of eigenvalues of the discretisation
\[
T^N_k := \begin{pmatrix} 0 & (\mathcal{D}^N_k)^{-1} \mathcal{Y}^N_- \\ (\mathcal{D}^N_k)^{-1} \mathcal{Y}^N_+ & 0 \end{pmatrix}^{-1}.
\]

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 \(T^N_k\) 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 $E_0(k, \alpha), \ldots, E_{40}(k, \alpha)$ of $H_k(\alpha)$ for $k^* = 1/(2\sqrt{3}) + i/6$ (see Figure 8). Numerous eigenvalues are quite close together or have high multiplicity.

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

To understand the accuracy of the values in Table 1, we studied $\|D_N^k(\alpha)^{-1}\|$ near the putative magic $\alpha$ values. Figure 8 reveals the computational challenge of resolving large magic angles to high fidelity. One can characterize the magic $\alpha$’s as points where $(D(\alpha) - k)^{-1}$ does not exist, and hence they are approximated by $\alpha$’s for which $\|D_N^k(\alpha)^{-1}\|$ is very large for generic $k$. Careful scanning for $\alpha$’s around magic values (using $N = 96$ and $N = 128$) refines the estimates and indicates their accuracy.
Table 1. Estimates of the first thirteen magic $\alpha$’s, truncated (not rounded) to digits supported with high confidence by our numerics. The last column shows the difference between consecutive magic $\alpha$’s, which seem to converge a bit above the conjecture of $3/2$ in [TKV19].

<table>
<thead>
<tr>
<th>$k$</th>
<th>$\alpha_k$</th>
<th>$\alpha_k - \alpha_{k-1}$</th>
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<tr>
<td>1</td>
<td>0.58566355838955</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2.2211821738201</td>
<td>1.6355</td>
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<tr>
<td>3</td>
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<td>1.5302</td>
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</tr>
<tr>
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<td>6.79478505720</td>
<td>1.5183</td>
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<tr>
<td>6</td>
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</tr>
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<td>7</td>
<td>9.829066969</td>
<td>1.5161</td>
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<td>8</td>
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</tr>
<tr>
<td>13</td>
<td>18.920</td>
<td>1.5147</td>
</tr>
</tbody>
</table>

Overall, as $\alpha$ increases $\|D_N^N(\alpha)^{-1}\|$ grows exponentially (as guaranteed by Theorem 4, since $\|D_N^N(\alpha)^{-1}\| = 1/E_0(k,\alpha)$), so that precisely locating large $\|D_N^N(\alpha)^{-1}\|$ values against this growing background becomes increasingly challenging. Indeed, this numerical struggle nicely parallels the presumed diminishing physical significance of large magic $\alpha$ values (corresponding, as they do, to reciprocals of angles of twisting).

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References


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