



Integrability in the Chiral Model of Magic Angles

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Received: 26 September 2022 / Accepted: 17 July 2023

Published online: 16 August 2023 – © The Author(s) 2023

Abstract: Magic angles in the chiral model of twisted bilayer graphene are parameters for which the chiral version of the Bistritzer–MacDonald Hamiltonian exhibits a flat band at energy zero. We compute the sums over powers of (complex) magic angles and use that to show that the set of magic angles is infinite. We also provide a new proof of the existence of the first real magic angle, showing also that the corresponding flat band has minimal multiplicity for the simplest possible choice of potentials satisfying all symmetries. These results indicate (though do not prove) a hidden integrability of the chiral model.

1. Introduction and Statement of Results

When two sheets of graphene are stacked on top of each other and twisted, it has been observed that at certain angles, coined the *magic angles*, the composite system becomes superconducting. In this article, we study the chiral limit of the Bistritzer–MacDonald Hamiltonian [1, 4, 5, 10]

$$H(\alpha) = \begin{pmatrix} 0 & D(\alpha)^* \\ D(\alpha) & 0 \end{pmatrix} \text{ with } D(\alpha) = \begin{pmatrix} D_z & \alpha U(z) \\ \alpha U(-z) & D_{\bar{z}} \end{pmatrix}$$

where the parameter α is proportional to the inverse relative twisting angle. After a simple rescaling, the potential is a smooth and periodic function satisfying

$$U(z + a_\ell) = \bar{\omega}U(z), \quad U(\omega z) = \omega U(z), \quad \text{and } U(\bar{z}) = \overline{U(z)}, \quad (1.1)$$

where $\omega = e^{2\pi i/3}$ and $a_\ell = \frac{4}{3}\pi i \omega^\ell$. The simplest example of such a potential and our canonical choice of U is

$$U_0(z) = \sum_{k=0}^2 \omega^k e^{\frac{1}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}. \quad (1.2)$$

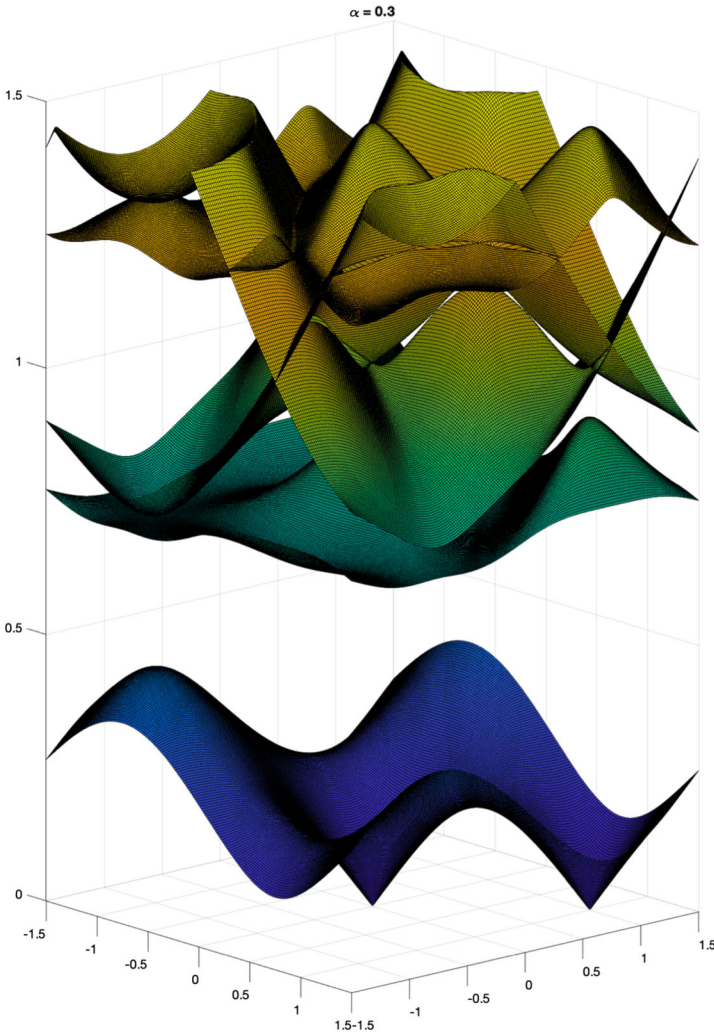


Fig. 1. Plots of the first 5 non-negative eigenvalues of $H_{\mathbf{k}}(0.3)$ acting on \mathcal{H} (see (1.4) and (1.5)), as function of $k = (k_1\omega^2 - k_2\omega)/\sqrt{3}$ in a fundamental cell of $3\Gamma^*$, parametrized by $(k_1, k_2) \mid |k_j| < \frac{3}{2}$. See also [3, Figure 4] for more information and comparison with band structure of other models

Even though the potential $U(z)$ is only periodic with respect to $\Gamma = 4\pi i(\omega\mathbb{Z} \oplus \omega^2\mathbb{Z})$ the first property implies that the matrix potential, and thus $D(\alpha)$, commutes with the translation operator

$$\mathcal{L}_a w(z) := \begin{pmatrix} \omega^{a_1+a_2} & 0 \\ 0 & 1 \end{pmatrix} w(z+a), \quad a \in \frac{1}{3}\Gamma, \tag{1.3}$$

where $w \in \mathbb{C}^2$ and $a = \frac{4}{3}\pi i(\omega a_1 + \omega^2 a_2)$, $a_j \in \mathbb{Z}$. We note that if Γ^* is the dual (reciprocal) lattice of Γ , then $3\Gamma^*$ is the dual lattice of $\frac{1}{3}\Gamma$ (Fig. 1).

When moving to functions with values in $\mathbb{C}^4 = \mathbb{C}^2 \times \mathbb{C}^2$ (on which $H(\alpha)$ acts) we extend the action of \mathcal{L}_a to an action on each \mathbb{C}^2 component. We then consider the

Floquet spectrum of

$$H_k(\alpha) = \begin{pmatrix} 0 & D(\alpha)^* - \bar{k} \\ D(\alpha) - k & 0 \end{pmatrix} \text{ with } k \in 3\Gamma^*, \tag{1.4}$$

defined by $(H_k(\alpha) - E_j(\alpha, k))w_j(\alpha, k) = 0$, where eigenvalues of positive energy are labelled with $j \geq 1$ in ascending order, as a self-adjoint operator on

$$\mathcal{H} := \{ \mathbf{v} \in L^2(\mathbb{C}/\Gamma) : \mathcal{L}_a \mathbf{v} = \mathbf{v}, \mathbf{a} \in \frac{1}{3}\Gamma \}, \tag{1.5}$$

with the domain given by $\mathcal{H} \cap H^1(\mathbb{C}/\Gamma)$ such that

$$\text{Spec}_{L^2(\mathbb{C}; \mathbb{C}^4)}(H(\alpha)) = \bigcup_{k \in \mathbb{C}} \text{Spec}_{\mathcal{H}}(H_k(\alpha)).$$

This Hamiltonian is an effective one-particle model which exhibits perfectly flat bands at magic angles. This appearance of perfectly flat bands in the chiral limit was explained by Tarnopolsky, Kruchkov and Vishwanath [9] with the help of Jacobi theta functions.¹ An equivalent spectral theoretic characterization of magic angles was then provided in [2]: if we define the following compact Birman–Schwinger operator

$$T_k = (2D_{\bar{z}} - k)^{-1} \begin{pmatrix} 0 & U(z) \\ U(-z) & 0 \end{pmatrix}. \tag{1.6}$$

then (see [2, Theorem 2]) we have the following equivalence [3, §2.3])

$$0 \in \bigcap_{k \in \mathbb{C}} \text{Spec}_{\mathcal{H}}(H_k(\alpha)) \iff \begin{cases} \alpha^{-1} \in \text{Spec}_{\mathcal{H}}(T_{k_0}) \\ \text{for some } k_0 \in \mathbb{C} \setminus (3\Gamma^* - \{0, i\}), \end{cases} \tag{1.7}$$

where \mathcal{H} is defined in (1.5). In other words, the spectrum of T_{k_0} is independent of $k_0 \in \mathbb{C} \setminus (3\Gamma^* - \{0, i\})$ and characterizes the values of $\alpha \in \mathbb{C}$ at which the Hamiltonian exhibits a flat band at zero energy. Since the parameter α is inherently connected with the twisting angle, we shall refer to α 's at which (1.7) occurs as *magic* and denote their set by $\mathcal{A} \subset \mathbb{C}$.

The analysis of magic angles is therefore reduced to a spectral theory problem involving a single compact non self-adjoint operator. Since even non-trivial non self-adjoint compact operators do not necessarily have non-zero eigenvalues, the existence of a parameter α at which the Hamiltonian exhibits a flat band at zero energy is non-trivial. In [2] the existence of such a complex parameter $\alpha \in \mathbb{C} \setminus \{0\}$ was first concluded by showing that $\text{tr}_{\mathcal{H}}(T_k^4) = 8\pi/\sqrt{3}$ which implied existence of a non-zero eigenvalue². This result was improved by a computer-assisted proof [11] in which Watson and Luskin used the complex-analytic characterization of magic angles from [9] to prove existence of the first *real* magic angle and obtained explicit bounds on its position.

In this article, we exhibit a general form of traces of powers of T_k . This suggests a hidden *integrability* of the Hamiltonian $H(\alpha)$ for potentials satisfying (1.1), as all traces exhibits special arithmetic properties. With our current techniques, we do not have explicit control on the full set of traces which would imply a complete understanding of all magic angles. These are already visible in the regular but evasive structure of the set of of magic α , $\mathcal{A} \subset \mathbb{C}$ —see Fig. 2.

¹ As was pointed out to us by Alex Sobolev a similar argument appeared in the work of Dubrovin and Novikov [6] who studied magnetic Hamiltonians on tori.

² In [2] we considered the trace on $L^2(\mathbb{C}/\Gamma; \mathbb{C}^2)$ which gave this answer multiplied by 9.

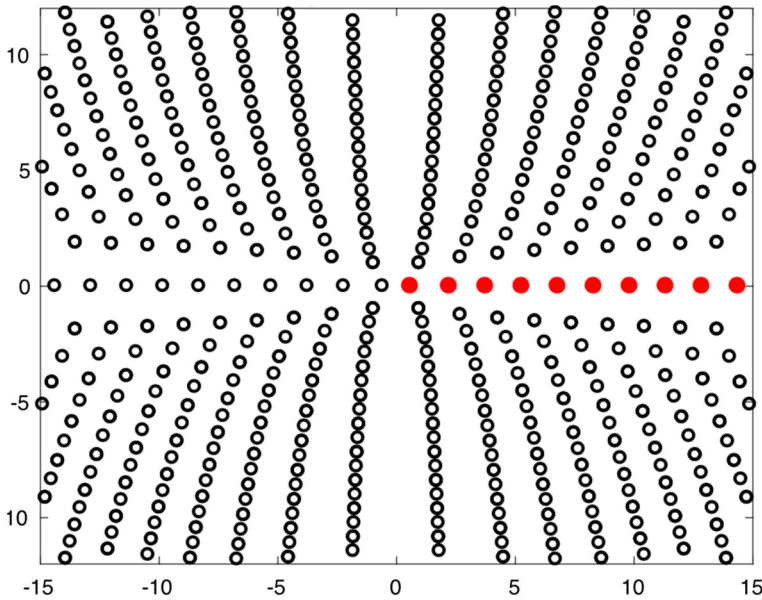


Fig. 2. The set \mathcal{A} of magic α 's for which (1.7) holds, that is, the first band is flat. The positive elements of \mathcal{A} are the reciprocals of the “physically relevant” positive angles. Potential (1.2) is responsible for the regularity of the set which seems to indicate hidden integrability. For more general potentials the distribution is more complicated—see <https://math.berkeley.edu/~zworski/multi.mp4> for $U_\theta(z) = (\cos^2 \theta)U(z) + (\sin^2 \theta) \sum_{k=0}^2 \omega^k e^{\bar{z}\omega^k} - z\bar{\omega}^k$ which satisfies the required symmetries (1.1). The animation also indicates changing multiplicities

Theorem 1. For $\ell \geq 2$ and $U = U_0$ with U_0 as in (1.2)

$$\text{tr}(T_k^{2\ell}) = \sum_{\alpha \in \mathcal{A}} \alpha^{-2\ell} = \frac{\pi}{\sqrt{3}} q_\ell \text{ with } q_\ell \in \mathbb{Q}. \tag{1.8}$$

In addition, we are able to express the rational numbers $q_\ell \in \mathbb{Q}$ in terms of a finite sum involving residues of rational functions which is fully presented in Theorem 4. A generalization of Theorem 1 which extends this result to more general potentials U (1.1) is presented in Theorem 5. As we show in Sect. 6, it is already possible to conclude directly from Theorem 1 that

Theorem 2. Let $U = U_0$ with U_0 as in (1.2). There exist infinitely many magic α 's, that is,

$$|\mathcal{A}| = \infty.$$

This theorem will follow from the more general Theorem 6 and the observation that by the aforementioned explicit computation $\text{tr}_{\mathcal{H}}(T_k^4) = 8\pi/\sqrt{3}$ for $U = U_0$ there is at least one complex magic angle. We then focus on real magic angles. Since the operator T_k^2 is Hilbert–Schmidt, we can use the regularized determinant to study real magic α . Compared with the initial approach proposed in [9], this approach has two advantages. Unlike the series expansion in [9, 11], the regularized determinant is an entire function with explicit error bounds in terms of the Hilbert–Schmidt norm. In addition, the Taylor coefficients of the determinant are polynomials of traces as in Theorem 1. This leads to

Theorem 3. *The chiral Hamiltonian with $U = U_0$ and U_0 as in (1.2), exhibits a flat band of multiplicity 2 at a real magic $\alpha_* \in (0.583, 0.589)$, which is minimal, in the sense that the Hamiltonian does not possess a flat band for any α satisfying $|\alpha| < |\alpha_*|$, that is,*

$$|\mathcal{A} \cap (0.583, 0.589)| = 1, \quad \mathcal{A} \cap D_{\mathbb{C}}(0, \alpha^*) = \emptyset,$$

where the counting $|\bullet|$ respects multiplicities. In particular, the flat bands of multiplicity 2 are uniformly gapped from all other bands.

Remark 1. Compared with results in [11] which require floating-point arithmetic, our proof of existence relies only on exact symbolic computations, the exact evaluation of residues to compute traces of powers of T_k and the summation of finitely many matrix entries to estimate the Hilbert-Schmidt norm.

2. Preliminaries

From now on, we consider a potential $U \in C^\infty(\mathbb{C}/\Gamma; \mathbb{C})$ satisfying the first two symmetries of (1.1). The last symmetry $U(\bar{z}) = \overline{U(z)}$ will only be needed in Corollary 5 to ensure that all traces are real. We recall that an orthonormal basis of $L^2(\mathbb{C}/\Gamma; \mathbb{C})$ is given by setting

$$e_\nu(z) := e^{\frac{i}{2}(\bar{\nu}z + \nu\bar{z})} / \sqrt{\text{Vol}(\mathbb{C}/\Gamma)}, \quad \nu \in \Gamma^* = \frac{1}{\sqrt{3}}(\mathbb{Z} + \omega\mathbb{Z}).$$

We can express the potential U in this basis. A straightforward calculation gives

Proposition 2.1. *Let $a = \frac{4\pi i}{3}(\omega a_1 + \omega^2 a_2) \in \Gamma/3$, $a_j \in \mathbb{Z}$. Then $u \in L^2(\mathbb{C}/\Gamma)$ satisfies*

$$u(z + a) = \bar{\omega}^{(a_1 + a_2)} u(z), \quad u(\omega z) = \omega u(z),$$

if and only if

$$u(z) = \sum_{n \in \mathbb{Z}^2} c_n e_{k_n} \tag{2.1}$$

where for $n \in \mathbb{Z}^2$

$$c_n = (u, e_{k_n})_{L^2(\mathbb{C}/\Gamma)}, \quad k_n = \frac{\omega^2(2 + 3n_1) - \omega(2 - 3n_2)}{\sqrt{3}},$$

satisfies

$$c_n = \omega c_{(-n_2)(n_1 - n_2 - 1)} = \omega^2 c_{(n_2 - n_1 + 1)(-n_1)}.$$

If in addition $\overline{u(\bar{z})} = u(z)$ then

$$\bar{c}_n = c_{(-n_2)(-n_1)} = \omega c_{n_1(n_1 - n_2 - 1)} = \omega^2 c_{(n_2 - n_1 - 1)n_2}.$$

Our aim is to obtain trace formulae for the powers of the compact operator T_k defined by in (1.6). Since odd powers of T_k have only off-diagonal components, it is clear that the traces of odd powers vanish. Thus, it is sufficient to compute the traces of powers of

$$T_k^2 = \begin{pmatrix} (2D_{\bar{z}} - k)^{-1}U(z)(2D_{\bar{z}} - k)^{-1}U(-z) & 0 \\ 0 & (2D_{\bar{z}} - k)^{-1}U(-z)(2D_{\bar{z}} - k)^{-1}U(z) \end{pmatrix}. \tag{2.2}$$

The invariance of the trace under cyclic permutations shows that it is sufficient to compute traces of powers of

$$\mathcal{A}_k := (2D_{\bar{z}} - k)^{-1}U(z)(2D_{\bar{z}} - k)^{-1}U(-z) : L^2(\mathbb{C}/\Gamma; \mathbb{C}) \rightarrow L^2(\mathbb{C}/\Gamma; \mathbb{C}), \quad k \notin \Gamma^*. \tag{2.3}$$

We shall study traces of powers of \mathcal{A}_k on smaller L^2 spaces, which we define below, for $(p_1, p_2) \in \mathbb{Z}_3^2$, by

$$L^2_{(p_1, p_2)}(\mathbb{C}/\Gamma; \mathbb{C}) := \left\{ u \in L^2 : u(z + 2i(\omega a_1 + a_2 \omega^2)) = e^{i(a_1 p_1 + a_2 p_2)} u(z); \right. \\ \left. a_j \in \frac{2\pi}{3}\mathbb{Z} \right\} \tag{2.4}$$

whose \mathbb{C}^2 -valued analogues are defined, using (1.3), as

$$L^2_{(p_1, p_2)}(\mathbb{C}/\Gamma; \mathbb{C}^2) := \left\{ u \in L^2 : \mathcal{L}_a u(z) = e^{i(a_1 p_1 + a_2 p_2)} u(z); a_j \in \frac{2\pi}{3}\mathbb{Z} \right\}. \tag{2.5}$$

We remark that the operator $(2D_{\bar{z}} - k)^{-1}$ acts diagonally on the Fourier basis and thus preserves the $L^2_{(p_1, p_2)}$ spaces. On the other hand, multiplication by $U(\pm z)$ does not preserve the space but one has by the translational symmetry defined in (1.1)

$$U(\pm z) : L^2_{(p_1, p_2)} \rightarrow L^2_{(p_1 \mp 1, p_2 \mp 1)}, \quad (p_1, p_2) \in \mathbb{Z}_3^2.$$

In total, we have

$$L^2_{(p_1, p_2)} \xrightarrow{U(-z)} L^2_{(p_1+1, p_2+1)} \xrightarrow{(2D_{\bar{z}}-k)^{-1}} L^2_{(p_1+1, p_2+1)} \xrightarrow{U(z)} L^2_{(p_1, p_2)} \xrightarrow{(2D_{\bar{z}}-k)^{-1}} L^2_{(p_1, p_2)}.$$

This shows that we can restrict the operator \mathcal{A}_k to the subspaces $L^2_{(p_1, p_2)}$. From now on, we will denote by A_k the restriction of \mathcal{A}_k to $L^2_{(1,1)}$. We then define the unitary multiplication operator

$$U_{(p_1, p_2)} : L^2_{(0,0)}(\mathbb{C}/\Gamma, \mathbb{C}^2) \rightarrow L^2_{(p_1, p_2)}(\mathbb{C}/\Gamma, \mathbb{C}^2), \\ U_{(p_1, p_2)} v(z) := e^{\frac{i}{2}(z\bar{p} + \bar{z}p)} v(z), \quad p = \frac{1}{\sqrt{3}}(\bar{\omega}p_1 - \omega p_2), \quad p_j \in \mathbb{Z}_3, \\ U_{(p_1, p_2)} T_k U_{(p_1, p_2)}^* = T_{k-p}, \quad k \notin \Gamma^*.$$

The k -independence of the spectrum of T_k implies then

$$\text{Spec}_{L^2_{(0,0)}(\mathbb{C}/\Gamma, \mathbb{C}^2)}(T_k^2) \setminus \{0\} = \text{Spec}_{L^2_{(1,1)}(\mathbb{C}/\Gamma, \mathbb{C}^2)}(T_k^2) \setminus \{0\} \\ = \text{Spec}_{L^2_{(1,1)}(\mathbb{C}/\Gamma, \mathbb{C})}(A_k) \setminus \{0\}, \tag{2.6}$$

where $k \in D(0, r) \setminus \{0\}$, and the last equality is meant in the sense of sets: multiplicities of elements in the top row are twice the multiplicities of elements in the bottom row.

We also note that A_k is defined for $k \in D(0, r)$ since $D_{\bar{z}}^{-1}$ is defined on $L^2_{(p,p)}$, $p \not\equiv 0 \pmod 3$. Since $\mathbb{C} \ni k \rightarrow \mathcal{A}_k|_{L^2_{(1,1)}}$ is an analytic family of operators with compact resolvents and the spectrum is independent of $k \in \mathbb{C} \setminus 3\Gamma^*$, it follows that $\text{Spec}(A_k) = \text{Spec}(A_0)$ [7, Theorem 1.10]. From (2.6) we obtain, as sets,

$$\text{Spec}_{L^2_{(0,0)}}(T_p^2) \setminus \{0\} = \text{Spec}_{L^2_{(1,1)}}(A_k) \setminus \{0\}, \quad p \in D(0, r) \setminus \{0\}, \quad k \in D(0, r), \quad (2.7)$$

with multiplicities on the left, twice the multiplicities on the right. Since $k = 0$ is included in the set of possible k for A_k . Indeed, the set of possible values of k is $\mathbb{C} \setminus ((3\Gamma^* - i) \cup (3\Gamma^* + i))$. We conclude together with [3, Theorem 2] that

$$\dim \ker_{\mathcal{H}}(D(\alpha)) = \dim \ker_{L^2_{(1,1)}}(A_0 - \alpha^{-2}). \quad (2.8)$$

We end this preliminary section by stating and proving the main three properties we will use for our calculation.

Lemma 2.2. *Consider a potential $U \in C^\infty(\mathbb{C}/\Gamma; \mathbb{C})$ satisfying the first two symmetries of (1.1) with a finite number of non zero Fourier mode in its decomposition (2.1). Define the operator A_k for $k \notin (3\Gamma^* - i) \cup (3\Gamma^* + i)$, where $i := -(\omega^2 - \omega)/\sqrt{3}$, to be the restriction of A_k defined in (2.3) on the space $L^2_{(1,1)}$. For $\ell \geq 2$, one has:*

- The trace is constant in k

$$\text{tr}(A_k^\ell) = \tau_\ell \text{ independent of } k \in \mathbb{C} \setminus (3\Gamma^* - i) \cup (3\Gamma^* + i). \quad (2.9)$$

- The function $\mathbb{C} \setminus (3\Gamma^* - i) \cup (3\Gamma^* + i) \ni k \mapsto \langle A_k^\ell e_m, e_m \rangle_{L^2}$ is a finite sum of rational fractions on the complex plane \mathbb{C} with degree equal to -2ℓ and with (a finite number of) poles contained in $(3\Gamma^* - i) \cup (3\Gamma^* + i)$.
- For any $\gamma \in \Gamma^*$ and for any $k \notin (3\Gamma^* - i) \cup (3\Gamma^* - 2i)$, we have

$$\langle A_k^\ell e_{3\gamma+i}, e_{3\gamma+i} \rangle_{L^2} = \langle A_{k-3\gamma}^\ell e_i, e_i \rangle_{L^2}.$$

Proof. The first point is a consequence of the independence of the spectrum of T_k in k (see [3, §2.3]) as well as the relation (2.7).

For the last two points, we prove by induction that $k \mapsto A_k^\ell e_{3\gamma+i}$, where $\gamma \in \Gamma^*$, is of the form

$$A_k^\ell e_{3\gamma+i} = \sum_{\nu \in F} R_{\nu+3\gamma}(k) e_{\nu+3\gamma}, \quad (2.10)$$

where $F \subset (3\Gamma^* + i)$ is a finite set and $R_\nu(k)$ is a sum of rational fraction of degree -2ℓ with poles located on $(3\Gamma^* - i) \cup (3\Gamma^* + i)$. Moreover, we will prove that the one has the relation $R_{\nu+3\gamma}(k) = R_\nu(k - 3\gamma)$.

The result is clear for $\ell = 0$. Suppose the result true for ℓ , let's prove it holds for $\ell + 1$. The main observation is that multiplication by $U(\pm z)$ acts as a shift on the Fourier basis. The multiplication by $U(-z)$ sends e_ν to a linear combination of e_ℓ for $\ell \in (3\Gamma^* + 2i)$. Then applying $(D(0) - k)^{-1}$ multiplies the coefficient of e_ℓ by $(\ell - k)^{-1}$. Multiplying by $U(z)$ gives back a linear combination of e_ν with $\nu \in (3\Gamma^* + i)$. Finally, applying

$(D(0) - k)^{-1}$ multiplies the coefficient of e_ν by $(\nu - k)^{-1}$. This means that, using the induction hypothesis (2.10),

$$A_k^{\ell+1} e_{3\gamma+i} = \sum_{\nu \in F} R_{\nu+3\gamma}(k) \sum_{\eta \in L} \sum_{\beta \in L} \frac{a_\eta}{k - (\nu + \beta - \eta + 3\gamma)} \frac{a_\beta}{k - (\nu + \beta + 3\gamma)} e_{\nu+\beta-\eta+3\gamma},$$

where $L \subset 3\Gamma^* + i$ is a finite subset that depends only on U and a_\bullet are constants. Thus, it is clear from this formula that the induction carries on to $\ell + 1$. This concludes the proof of the Lemma. \square

3. Trace Computations

We prove the following result.

Theorem 4. *Let $A_k : L^2_{(1,1)} \rightarrow L^2_{(1,1)}$ be a meromorphic family of Hilbert–Schmidt operators defined for $k \notin (3\Gamma^* - i) \cup (3\Gamma^* + i)$. We suppose that A_k satisfies the three properties stated in Lemma 2.2. Then one has, for any $\ell \geq 2$,*

$$\begin{aligned} \tau_\ell = \frac{2i\pi\omega}{3\sqrt{3}} \sum_{n \in \mathbb{Z}} n \left[\sum_{m \in \mathbb{Z}} \text{Res}(\langle A_k^\ell e_i, e_i \rangle_{L^2}, \sqrt{3}(m\omega^2 - n\omega) + i) \right. \\ \left. + \sum_{m \in \mathbb{Z}} \text{Res}(\langle A_k^\ell e_i, e_i \rangle_{L^2}, \sqrt{3}(m\omega^2 - n\omega) + 2i) \right], \end{aligned} \tag{3.1}$$

where all the infinite sums are in fact finite.

Proof. We want to give a semi-explicit formula for τ_ℓ in terms of the residue of the rational fraction (second point in Lemma 2.2)

$$k \in \mathbb{C} \setminus (3\Gamma^* - i) \cup (3\Gamma^* + i) \mapsto \langle A_k^\ell e_i, e_i \rangle_{L^2}.$$

We first start by writing, using that A_k^ℓ is trace-class for $\ell \geq 2$,

$$\tau_\ell = \sum_{\gamma \in \Gamma} \langle A_k^\ell e_{3\gamma+i}, e_{3\gamma+i} \rangle_{L^2}.$$

We start with the relation which follows directly from (2.9),

$$3\tau_\ell = \int_0^3 \text{tr} (A_{t\omega^2/\sqrt{3}}^\ell) dt = \int_0^3 \sum_{n \in \mathbb{Z}^2} \langle A_{t\omega^2/\sqrt{3}}^\ell e_{3\gamma_n+i}, e_{3\gamma_n+i} \rangle_{L^2} dt.$$

Here, we wrote $\gamma_n := \frac{1}{\sqrt{3}}(n_1\omega^2 - n_2\omega) \in \Gamma^*$. We now use the third property stated in Lemma 2.2 to write

$$3\tau_\ell = \int_0^3 \sum_{n \in \mathbb{Z}^2} \langle A_{t\omega^2/\sqrt{3}-3\gamma_n}^\ell e_i, e_i \rangle_{L^2} dt.$$

The second property in Lemma 2.2 implies that

$$\langle A_k^\ell e_i, e_i \rangle_{L^2} = \mathcal{O}(k^{-2\ell}). \tag{3.2}$$

Since we assume that $\ell \geq 2$, this justifies the exchange of integration and summation such that

$$3\tau_\ell = \sum_{n \in \mathbb{Z}^2} \int_0^3 \langle A_{(t+3n_1)\omega^2/\sqrt{3}-3n_2\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} dt.$$

We make the change of variable $s = t + 3n_1$ and sum in n_1 to get

$$3\tau_\ell = \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3n\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} dt. \tag{3.3}$$

We now consider

$$\int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3n\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} dt - \int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3(n+1)\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} dt, \quad n \in \mathbb{Z}.$$

This is equal to the limit of the integral over a parallelogram $\Gamma_{n,R}$ with sides $\frac{1}{\sqrt{3}}[-R\omega^2 - 3n\omega, R\omega^2 - 3n\omega]$, $\frac{1}{\sqrt{3}}[R\omega^2 - 3n\omega, R\omega^2 - 3(n+1)\omega]$, $\frac{1}{\sqrt{3}}[R\omega^2 - 3(n+1)\omega, -R\omega^2 - 3(n+1)\omega]$ and $\frac{1}{\sqrt{3}}[-R\omega^2 - 3(n+1)\omega, -R\omega^2 - 3n\omega]$. Here, we used (3.2) to prove that the integral over the small parallel sides tends to 0. In particular, because there is only a finite number of poles, we see that, for $|n|$ large enough, one has

$$\int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3n\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} dt - \int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3(n+1)\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} dt = 0.$$

Using formula (3.3) as well as a partial summation, this allows us to rewrite the full trace as a telescopic sum

$$3\tau_\ell = \sum_{n \in \mathbb{Z}} n \left[\int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3n\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} dt - \int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3(n+1)\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} dt \right]. \tag{3.4}$$

The residue theorem shows that for $n \in \mathbb{Z}$ and R large enough,

$$\int_{\Gamma_{n,R}} \langle A_z^\ell e_i, e_i \rangle_{L^2} dz = \int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3n\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} \frac{\omega^2}{\sqrt{3}} dt - \int_{\mathbb{R}} \langle A_{t\omega^2/\sqrt{3}-3(n+1)\omega/\sqrt{3}}^\ell e_i, e_i \rangle_{L^2} \frac{\omega^2}{\sqrt{3}} dt. \tag{3.5}$$

Applying the residue theorem and using (3.4) gives (3.1). \square

The consequences of this formula are summarized in the following theorem:

Theorem 5. Consider a potential $U \in C^\infty(\mathbb{C}/\Gamma; \mathbb{C})$ satisfying the first two symmetries of (1.1) with finitely many non-zero Fourier modes $c_n \in \mathbb{Q}(\omega/\sqrt{3})$ appearing in the decomposition (2.1). Then for any $\ell \geq 2$, one has $\tau_\ell \in \pi\mathbb{Q}(\omega/\sqrt{3})$. If U also has the third symmetry of (1.1) then the traces are real and thus $\tau_\ell \in \pi\mathbb{Q}/\sqrt{3}$. In particular,

for all potentials satisfying all three symmetries in (1.1), including $U = U_0$ defined in (1.2), one has

$$\forall \ell \geq 2, \quad \text{tr}(T_k^{2\ell}) = \sum_{\alpha \in \mathcal{A}(U)} \alpha^{-2\ell} = \frac{\pi}{\sqrt{3}} q_\ell, \quad q_\ell \in \mathbb{Q},$$

where $\mathcal{A}(U)$ is the set of magic angles counting multiplicity for a potential U .

Proof. Under the hypothesis of the corollary, the function $k \mapsto \langle A_k^\ell e_i, e_i \rangle_{L^2}$ is a rational fraction with coefficients in $\mathbb{Q}(\omega/\sqrt{3})$. This ring is actually a field as $\omega/\sqrt{3}$ is algebraic on \mathbb{Q} . Now, taking partial fraction expansion of $k \mapsto \langle A_k^\ell e_i, e_i \rangle_{L^2}$ in $\mathbb{Q}(\omega/\sqrt{3})(X)$ (the space of rational fractions with coefficients living in $\mathbb{Q}(\omega/\sqrt{3})(X)$) gives coefficients in $\mathbb{Q}(\omega/\sqrt{3})$. In particular, the residues of $k \mapsto \langle A_k^\ell e_i, e_i \rangle_{L^2}$ live in the field $\mathbb{Q}(\omega/\sqrt{3})(X)$. But the uniqueness of the partial fraction expansion now gives that these are also the residues of $k \mapsto \langle A_k^\ell e_i, e_i \rangle_{L^2}$ in $\mathbb{C}(X)$. Using the trace formula stated in Theorem 4, this yields

$$\forall \ell \geq 2, \quad \tau_\ell \in \pi \mathbb{Q}(\omega/\sqrt{3}).$$

If we add the last symmetry of (1.1), the trace is real so that

$$\forall \ell \geq 2, \quad \tau_\ell \in \pi \mathbb{Q}(\omega/\sqrt{3}) \cap \mathbb{R} \Rightarrow \tau_\ell = \frac{\pi}{\sqrt{3}} q_\ell, \quad q_\ell \in \mathbb{Q}.$$

□

This rationality condition suffices to prove that there is an infinite number of magic angles as long as there exists at least one magic angle.

Theorem 6. *Under the assumptions and with the same notation as in Theorem 5 one has the implication*

$$|\mathcal{A}(U)| > 0 \Rightarrow |\mathcal{A}(U)| = +\infty.$$

In particular, the set of magic angles for our canonical potential U_0 defined in (1.2) is infinite.

Let $N \geq 0$, for a tuple $a = (a_n)_{\{n; \|n\|_\infty \leq N\}}$, define U_a to be the potential defined by (2.1). Then the above implication holds for a generic (in the sense of Baire) set of coefficients $a = (a_n)_{\{n; \|n\|_\infty \leq N\}} \in \mathbb{C}^{(2N+1)^2}$ that contains $(\mathbb{Q}(\omega/\sqrt{3}))^{(2N+1)^2}$.

Proof. We start by observing that since π is transcendental on \mathbb{Q} , it is also transcendental in $\mathbb{Q}(\omega/\sqrt{3})$. Now, assume by contradiction, that there exist only finitely many eigenvalues $\lambda_i \in \mathbb{C}$ for $i = 1, \dots, N$ of A_k^2 . Then we define the n -th symmetric polynomial

$$e_n(\lambda_1, \dots, \lambda_N) = \sum_{1 \leq j_1 < j_2 < \dots < j_n \leq N} \lambda_{j_1} \cdots \lambda_{j_n}.$$

Newton identities show that this polynomial can be expressed as

$$e_n(\lambda_1, \dots, \lambda_N) = (-1)^n \sum_{\substack{m_1+2m_2+\dots+nm_n=n \\ m_1 \geq 0, \dots, m_n \geq 0}} \prod_{i=1}^n \frac{(-\text{tr } A_k^{2i})^{m_i}}{m_i! i^{m_i}} \tag{3.6}$$

where $e_n = 0$ for $n > N$. Theorem 1 shows that

$$\prod_{i=1}^n (\text{tr } A_k^{2i})^{m_i} \in \mathbb{Q} \left(\frac{\omega}{\sqrt{3}} \right) \pi^{m_1 \cdots m_n}.$$

The power $m_1 \cdots m_n$ from sequences allowed in (3.6) is maximized by the unique choice $m = (n, 0, \dots, 0)$. The Newton identities for $n > N$ then imply that the transcendental number π is a root of a polynomial with coefficients in $\mathbb{Q}(\omega/\sqrt{3})$. But then all these coefficients vanish, this is equivalent to the fact that the spectrum is empty (because of the determinant function, see (4.4)). For our particular choice of potential U_0 , the fact that $\text{tr } A_k^2 = 0$ contradicts [2, Theorem 3] so the set of magic angles is non empty, and thus infinite.

Now, let $a = (a_n)_{\{n; \|n\|_\infty \leq N\}} \in \mathbb{C}^{(2N+1)^2}$ and assume that $\mathcal{A}(U_a) \neq \emptyset$. Then, we can find an open neighbourhood of a , $\Omega_a \ni a$, such that for coefficients $b = (b_n)_{\{n; \|n\|_\infty \leq N\}} \in \Omega_a$ we have $\mathcal{A}(U_b) \neq \emptyset$. Take $q = (q_n)_{\{n; \|n\|_\infty \leq N\}} \in (\mathbb{Q}(\omega/\sqrt{3}))^{(2N+1)^2} \cap \Omega_a$ for which we then have $|\mathcal{A}(U_q)| = \infty$. Continuity of eigenvalues of T_k as the potential U changes shows that the $V_{m,a} := \{b \in \Omega_a : |\mathcal{A}(U_b)| \geq m\}$ is open and dense in Ω_a . Hence, the set coefficients for which $0 < |\mathcal{A}_b| < \infty$ is given by $\bigcup_{m \in \mathbb{N}} \bigcup_{q \in (\mathbb{Q}+i\mathbb{Q})^{2N+1}} \Omega_q \setminus V_{m,q}$. It is then meagre and does not contain $(\mathbb{Q}(\omega/\sqrt{3}))^{(2N+1)^2}$. \square

4. Fredholm Determinants and the First Magic Angle

In this section, we explain how to compute the first few traces from our formula and show the existence of a simple real magic angle, i.e. prove Theorem 3. From now on, our choice of potential is given by $U = U_0$ defined in 1.2. Here we recall some facts from [2,3] needed in this paper.

4.1. *Fourier coordinates.* For our numerics, it is convenient to use rectangular coordinates $z = 2i(\omega y_1 + \omega y_2)$, see [2, §3.3] for details. In these coordinates, we may introduce

$$\begin{aligned} \mathcal{D}_k &:= \omega^2(D_{y_1} + k_1) - \omega(D_{y_2} + k_2), \\ \mathcal{V}(y) &:= \sqrt{3}(e^{-i(y_1+y_2)} + \omega e^{i(2y_1-y_2)} + \omega^2 e^{i(-y_1+2y_2)}), \end{aligned} \tag{4.1}$$

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 $\mathcal{V}_\pm(y) := \mathcal{V}(\pm y)$. The operator \mathcal{A}_k , defined in (2.3), reads in the new coordinates

$$\mathcal{D}_k^{-1} \mathcal{V}_+ \mathcal{D}_k^{-1} \mathcal{V}_- : L^2(\mathbb{C}/2\pi(\mathbb{Z} + i\mathbb{Z}); \mathbb{C}) \rightarrow L^2(\mathbb{C}/2\pi(\mathbb{Z} + i\mathbb{Z}); \mathbb{C}).$$

On the Fourier transform side we introduce the equivalent of operators (4.1)

$$\begin{aligned} \widehat{\mathcal{D}}_k &:= \omega^2(D + k_1) - \omega(D + k_2), \text{ with } D = \text{diag}(\ell)_{\ell \in \mathbb{Z}} \\ \widehat{\mathcal{V}}_\pm(y) &:= \sqrt{3} \left(J^\pm \otimes J^\pm + \omega J^{\mp 2} \otimes J^\pm + \omega^2 J^\pm \otimes J^{\mp 2} \right), \end{aligned} \tag{4.2}$$

where J is the right-shift $J((a_n)_n) = (a_{n+1})_n$ —see [2, (3.17)]. The spaces $L^2_{(p_1, p_2)}(\mathbb{C}/\Gamma; \mathbb{C})$, introduced in (2.4), correspond to

$$\ell^2_{(p_1, p_2)} := \{f \in \ell^2(\mathbb{Z}^2) : \forall n \notin (3\mathbb{Z} + p_1) \times (3\mathbb{Z} + p_2), f_n = 0\}.$$

As in [2, §3.3], we introduce auxiliary operators $J^{p, q} := J^p \otimes J^q$, $p, q \in \mathbb{Z}$. For a diagonal matrix $\Lambda = (\Lambda_{i, j})_{i, j \in \mathbb{Z}}$ acting on $\ell^2(\mathbb{Z}^2)$, we define a new diagonal matrix

$$\Lambda_{p, q} := (\Lambda_{i+p, j+q})_{i, j \in \mathbb{Z}}.$$

We recall the following properties [2, (3.24)]

$$J^{p, q} \Lambda J^{p', q'} = \Lambda_{p, q} J^{p+p', q+q'} = J^{p+p', q+q'} \Lambda_{-p', -q'}. \tag{4.3}$$

Denoting the inverse of $\widehat{\mathcal{D}}_k^{-1}$ by

$$\Lambda = \Lambda_k := \widehat{\mathcal{D}}_k^{-1}, \quad \Lambda_{m, n} = \frac{1}{\omega^2(m + k_1) - \omega(n + k_2)}, \quad (k_1, k_2) \notin \mathbb{Z}^2,$$

we see that \mathcal{A}_k reads in the new Fourier coordinates

$$\begin{aligned} \frac{1}{3} \widehat{\mathcal{A}}_k &= \Lambda \Lambda_{1,1} + \omega \Lambda \Lambda_{1,-2} + \omega^2 \Lambda \Lambda_{-2,1} + \omega \Lambda \Lambda_{1,1} J^{3,0} + \omega^2 \Lambda \Lambda_{1,1} J^{0,3} \\ &\quad + \omega \Lambda \Lambda_{-2,1} J^{-3,0} + \omega^2 \Lambda \Lambda_{1,-2} J^{0,-3} + \Lambda \Lambda_{-2,1} J^{-3,3} + \Lambda \Lambda_{1,-2} J^{3,-3} \end{aligned}$$

with \widehat{A}_k the analogous restriction to $\ell^2_{(1,1)}$.

4.2. *Fredholm determinants.* We start by defining the regularized Fredholm determinant

$$\det_2(1 - \alpha^2 \widehat{A}_k) = \prod_{\lambda \in \text{Spec}(A_k)} E_1(\alpha^2 \lambda) \text{ with } E_1(z) = (1 - z)e^z \tag{4.4}$$

where the product respects multiplicities. We find from (2.6) that $\det_2(1 - \alpha^2 \widehat{A}_k) = 0 \Leftrightarrow \alpha^{-1} \in \text{Spec}(T_k) \setminus \{0\}$. The symmetry of the spectrum of \widehat{A}_k , $\text{Spec}(\widehat{A}_k) = \overline{\text{Spec}(\widehat{A}_k)}$, implies that $\alpha \mapsto \det_2(1 - \alpha^2 \widehat{A}_k)$ is real-valued on the real axis. To show existence and simplicity of magic angles, in the representation, we therefore use the following Lemma which provides ab initio bounds on the Fredholm determinants and its derivatives.

Lemma 4.1. *The determinant $\mathbb{C} \ni \alpha \mapsto \det_2(1 - \alpha^2 \widehat{A}_k)$ in (4.4) is an entire function, independent of $k \in \mathbb{C}$, which for any $n, m \in \mathbb{N}_0$ satisfies*

$$\left| \partial_\alpha^m \det_2(1 - \alpha^2 \widehat{A}_k) - \partial_\alpha^m \sum_{j=0}^n \mu_j \frac{(-\alpha^2)^j}{j!} \right| \leq \sum_{j=n+1}^\infty \partial_{|\alpha|}^m \left(\frac{\sqrt{e} \inf_{k \in \mathbb{C}} \|\widehat{A}_k\|_2 |\alpha|^2}{\sqrt{j}} \right)^j$$

with $\|A_0\|_2 \leq 2$, where

$$\mu_j := \det \begin{pmatrix} 0 & j-1 & 0 & \cdots & 0 \\ \sigma_2 & 0 & j-2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \sigma_{j-1} & \sigma_{j-2} & \cdots & 0 & 1 \\ \sigma_j & \sigma_{j-1} & \sigma_{j-2} & \cdots & 0 \end{pmatrix}, \text{ with } \sigma_j = \text{tr } \widehat{A}_k^j. \tag{4.5}$$

Proof. The expression (4.4) is well-defined since \widehat{A}_k is a Hilbert-Schmidt operator and the Taylor coefficients μ_j are for example stated in [8, (6.13)]. Indeed, since $|E_1| \leq e^{\frac{|z|^2}{2}}$ for $z \in \mathbb{C}$ and $\sum_{\lambda \in \text{Spec}(\widehat{A}_k)} |\lambda|^2 \leq \|\widehat{A}_k\|_2^2$, we conclude that

$$|\det_2(1 - \alpha^2 \widehat{A}_k)| \leq \exp\left(\frac{|\alpha|^4 \|\widehat{A}_k\|_2^2}{2}\right). \tag{4.6}$$

Cauchy estimates for the entire function $f(z) := \det_2(1 + z \widehat{A}_k)$ show by using the growth bound (4.6)

$$|\mu_j| \leq \frac{j!}{|\alpha|^{2j}} \exp\left(\frac{|\alpha|^4 \|\widehat{A}_k\|_2^2}{2}\right)$$

which is optimized at $|\alpha|^2 = \frac{\sqrt{j}}{\|\widehat{A}_k\|_2}$, such that

$$|\mu_j| \leq \frac{\|\widehat{A}_k\|_2^j e^{j/2} j!}{j^{j/2}}.$$

The Taylor coefficients μ_j are then given by the Plemelj-Smithies formula [8] stated in (4.5). Since they only depend on traces σ_j which are independent of k , it follows that the regularized Fredholm determinant is an entire function independent of k . Hence, it suffices to study the determinant for $k = 0$.

If we write $\widehat{A}_0 = (\widehat{A}_0(n))_{n \in \mathbb{Z}^2}$ and let P_m be the projection onto $(3\{-m, -m + 1, \dots, m\} + 1)^2$, then

$$\|\widehat{A}_0\|_2 \leq \|P_M \widehat{A}_0\|_2 + \|(\text{id} - P_M) \widehat{A}_0\|_2. \tag{4.7}$$

The first term constitutes the Hilbert-Schmidt norm of a finite matrix which can be explicitly computed from the matrix elements using symbolic calculations, indeed

$$\|P_M \widehat{A}_0\|_2 = \sqrt{\text{tr}(P_M \widehat{A}_0 \widehat{A}_0^* P_M)} \leq 5 \text{ for } M = 760.$$

To estimate the second term, we may use that the operator norm of \mathcal{V}_\pm satisfies $\|\mathcal{V}_\pm\| = 3\sqrt{3}$, therefore one has

$$\|(\text{id} - P_M) \widehat{A}_0\|_2 \leq 9 \|(\text{id} - P_M) (\mathcal{D}_0^{-1})_{\ell_{(1,1)}^2 \rightarrow \ell_{(1,1)}^2}\|_4 \|(\mathcal{D}_0^{-1})_{\ell_{(2,2)}^2 \rightarrow \ell_{(2,2)}^2}\|_4. \tag{4.8}$$

We recall that by definition

$$\|(\mathcal{D}_0^{-1})_{\ell_{(1,1)}^2 \rightarrow \ell_{(1,1)}^2}\|_4 = \left(\sum_{m \in (3\mathbb{Z}+1)^2} |\omega^2 m_1 - \omega m_2|^{-4} \right)^{1/4}.$$

A simple change of variables shows that $\|(\mathcal{D}_0^{-1})_{\ell_{(1,1)}^2 \rightarrow \ell_{(1,1)}^2}\|_4 = \|(\mathcal{D}_0^{-1})_{\ell_{(2,2)}^2 \rightarrow \ell_{(2,2)}^2}\|_4$. Then, a direct computation shows that in terms of

$$g(m) = \frac{3((m_1 + 1)^2 + (m_2 + 1)^2 + (m_1 + m_2)^2)}{2} - 2$$

we have

$$\|(\mathcal{D}_0^{-1})_{\ell^2_{(2,2)} \rightarrow \ell^2_{(2,2)}}\|_4 = \frac{1}{\sqrt{3}} \left(\sum_{m \in \mathbb{Z}^2} \frac{1}{g(m)^2} \right)^{1/4}.$$

While an explicit computation shows using exact symbolic calculations

$$\sum_{|m|_\infty \leq 6} \frac{1}{g(m)^2} \leq \frac{24}{7} \tag{4.9}$$

Then, we may use for $|m|_\infty > 6$ that $g(m) \geq |m|^2 + 5^2$, such that we can estimate the remainder

$$\begin{aligned} \sum_{|m|_\infty \geq 7} \frac{1}{g(m)^2} &\leq \int_6^\infty \frac{2\pi r}{(r^2 + 5^2)^2} dr = \frac{\pi}{61} \\ \Rightarrow \|(\mathcal{D}_0^{-1})_{\ell^2_{(2,2)} \rightarrow \ell^2_{(2,2)}}\|_4 &\leq \left(\frac{8}{21} + \frac{\pi}{549} \right)^{1/4}. \end{aligned} \tag{4.10}$$

Inserting this estimate into (4.8), we find along the lines of (4.10)

$$\begin{aligned} \|(\text{id} - P_M)\widehat{A}_0\|_2 &\leq \frac{213}{10} \|(\text{id} - P_M)(\mathcal{D}_0^{-1})_{\ell^2_{(1,1)} \rightarrow \ell^2_{(1,1)}}\|_4 \\ &\leq \frac{213}{10} \frac{1}{\sqrt{3}} \left(\int_{760}^\infty \frac{2\pi r}{(r^2 + 759^2)^2} dr \right)^{1/4} < \frac{1}{2}, \end{aligned} \tag{4.11}$$

which shows that $\|\widehat{A}_0\|_2 < \frac{1}{2}$. □

Using the preceding error estimate with the explicit traces in Table 1, we conclude the existence of a first real magic angle in the next Proposition. The Proposition also completes the proof of Theorem 3. Indeed, (2.8) implies together with [3, Theorem 2] the existence of a 0 gap between the two flat bands of the Hamiltonian and the remaining bands.

Proposition 4.2. *There exists a simple real eigenvalue $\frac{1}{\alpha_*}$ to the operator \widehat{A}_k , independent of $k \in \mathbb{C}$, with $\alpha_* \in (0.583, 0.589)$ such that $(\frac{1}{\alpha_*}, \infty) \subset \mathbb{R} \setminus \text{Spec}(\widehat{A}_k)$.*

Proof. To see that this is the first real magic angle, we first notice that the operator norm of \widehat{A}_0 is bounded by

$$\|\widehat{A}_0\| \leq (3\sqrt{3})^2 \|(\mathcal{D}_0^{-1})_{\ell^2_{(1,1)} \rightarrow \ell^2_{(1,1)}}\|^2 = 9.$$

This estimate shows that $\alpha \in \mathbb{R}^+$ with $1/(\alpha^2) \in \text{Spec}(\widehat{A}_0)$ satisfies $\alpha \geq \frac{1}{3}$. A finite number of traces as explicitly computed in Table 1 are then relevant to prove the existence of a magic angle.

For $\nu \in \mathbb{R}^+$ we find

$$r_i \leq \left(\frac{2\nu}{\alpha} \right)^i \frac{\left(\frac{\nu}{\sqrt{N}} \right)^{N-i}}{1 - \frac{\nu}{\sqrt{N}}} \text{ for } r_0 := \sum_{k=N}^\infty \left(\frac{\nu}{\sqrt{k}} \right)^k \text{ and } r_1 := \sum_{k=N}^\infty \frac{2k}{\alpha} \left(\frac{\nu}{\sqrt{k}} \right)^k.$$

Table 1. First eight exact traces of A_k^p , $\sigma_p = \text{tr}(A_k^p)$, with floating point approximation, where $\sigma_1 := \lim_{n \rightarrow \infty} \sum_{|i| \leq n} \langle A_k e_i, e_i \rangle$ is not absolutely summable as A_k is not of trace-class, computed using Theorem 4 in the version stated as Theorem 7 in the appendix. One sees that the ratio of $\sigma_p/\sigma_{p-1} \approx 1/0.5857^2 = 2.91507$, for p large, where 0.5857 is the first magic angle

p	$\sigma_p \frac{\sqrt{3}}{\pi}$
1	$2/3$
2	4
3	$96/7 \approx 13.71$
4	40
5	$28680/247 \approx 116.14$
6	$2206080/6517 \approx 338.51$
7	$1957475168/1983163 \approx 987.05$
8	$39948260880/13882141 \approx 2877.67$

Evaluating the bound for $N = 17$ and $v = \sqrt{e} \|\widehat{A}_0\|_2 \alpha^2$, as in the error bound stated in Lemma 4.1, with upper bound $\|\widehat{A}_0\|_2 = 5.5$, we obtain for $\alpha = \frac{3}{5}$ that $r_0 \leq \frac{1}{50}$ and $r_1 \leq \frac{1}{2}$. The existence of a root follows from studying

$$f(\alpha) := \sum_{k=0}^{16} \mu_k \frac{(-\alpha^2)^k}{k!}, \quad \sup_{\alpha \in (1/3, \beta)} f'(\alpha) \leq g(\beta = 0.6) := \sum_{k=2}^{20} a_k(\beta),$$

where the summation starts at $k = 2$ since $\mu_1 = 0$, with

$$a_k(\beta) = \begin{cases} 2\mu_k \frac{(-1)^k \left(\frac{1}{3}\right)^{2k-1}}{(k-1)!}, & \text{if } \mu_k(-1)^k < 0 \\ 2\mu_k \frac{(-1)^k \left(\frac{3}{5}\right)^{2k-1}}{(k-1)!}, & \text{if } \mu_k(-1)^k \geq 0. \end{cases}$$

One then checks (using computations involving integers only)

$$f(0.583) > \frac{1}{40}, \quad f(0.589) < -\frac{1}{40}, \quad \text{and } g\left(\frac{3}{5}\right) < -\frac{7}{10}.$$

We conclude that there is $\alpha_* \in (0.583, 0.589)$ such that $\det_2(1 - \alpha_*^2 \widehat{A}_k) = 0$ and $\partial_\alpha|_{\alpha=\alpha_*} \det_2(1 - \alpha^2 \widehat{A}_k) < 0$. The non-existence of any other $\alpha \in (\frac{1}{3}, \alpha_*)$ at which the determinant vanishes follows from the monotonicity of f . \square

Acknowledgements We would like to thank the two anonymous referees for their careful reading of the paper and many helpful comments. TH and MZ gratefully acknowledge partial support by the National Science Foundation under the Grant DMS-1901462 and by the Simons Foundation Targeted Grant Award No. 896630.

Funding Open access funding provided by Swiss Federal Institute of Technology Zurich

Declarations

Conflict of interest The authors have no competing interests to declare that are relevant to the content of this article.

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Appendix: Trace Formula in Fourier Coordinates

In this section we give an auxiliary version of Theorem 4 that we used for our computer assisted computation of traces. Using the relation (4.3), the diagonal part of \mathcal{A}_k^ℓ is of the form

$$\begin{aligned}
 ((\mathcal{A}_k^\ell)_{ii})_{i \in \mathbb{Z}} &= 3^\ell \sum_{\pi \in \Theta_\ell} \omega^{m_\pi} \prod_{i=1}^\ell \Lambda_{\tilde{\alpha}_i, \tilde{\beta}_i} \Lambda_{\tilde{\gamma}_i, \tilde{\delta}_i}, \\
 \pi &:= [(\alpha_1, \beta_1), (\gamma_1, \delta_1), (\alpha_2, \beta_2), \dots, (\gamma_\ell, \delta_\ell)],
 \end{aligned}
 \tag{A.1}$$

where

$$\begin{aligned}
 \tilde{\alpha}_i &= \sum_{j=1}^{i-1} \alpha_j + \gamma_j & \tilde{\beta}_i &= \sum_{j=1}^{i-1} \beta_j + \delta_j, & \tilde{\gamma}_i &= \alpha_i + \sum_{j=1}^{i-1} \alpha_j + \gamma_j, \\
 \tilde{\delta}_i &= \beta_i + \sum_{j=1}^{i-1} \beta_j + \delta_j, & m_\pi &:= \frac{2}{3} \sum_{i=1}^\ell (\gamma_i + \beta_i).
 \end{aligned}
 \tag{A.2}$$

In (A.1), the sum is over elements of the finite set

$$\begin{aligned}
 \Theta_\ell &:= \left\{ \pi = [(\alpha_1, \beta_1), (\gamma_1, \delta_1), (\alpha_2, \beta_2), \dots, (\gamma_\ell, \delta_\ell)], \sum_{j=1}^\ell \alpha_j + \gamma_j = \sum_{j=1}^\ell \beta_j + \delta_j = 0, \right. \\
 &\quad \left. (\alpha_i, \beta_i) \in \{(1, 1), (-2, 1), (1, -2)\}, (\gamma_i, \delta_i) \in \{(-1, -1), (2, -1), (-1, 2)\} \right\}.
 \end{aligned}
 \tag{A.3}$$

Using (A.1), the diagonal part of A_k^ℓ , is of the form

$$3^\ell \sum_{\pi \in \Theta_\ell} \omega^{m_\pi} \prod_{i=1}^\ell \Lambda'_{\alpha_i, \beta_i} \Lambda'_{\gamma_i, \delta_i}, \quad \pi = [(\alpha_1, \beta_1), (\gamma_1, \delta_1), (\alpha_2, \beta_2), \dots, (\gamma_\ell, \delta_\ell)],$$

where Λ' corresponds to the matrix where we only kept the coefficients (n, m) where $(n, m) \in (3\mathbb{Z} + 1) \times (3\mathbb{Z} + 1)$ i.e

$$\Lambda'_{m,n} = \frac{1}{\omega^2(3m + 1 + k_1) - \omega(3n + 1 + k_2)}.$$

Theorem 4 then reduces to

Theorem 7. Let $\ell \geq 2$ and Θ_ℓ be as in (A.3) with coefficients $\tilde{\alpha}_i, \dots, \tilde{\delta}_i, m_\pi$ as in (A.2). Then the traces are given by

$$\text{tr} \left(A_k^\ell \right) = -\frac{2i\omega\pi}{3} \sum_{\pi \in \Theta_\ell} \sum_{(\eta_i, \epsilon_i) \in \{(\tilde{\alpha}_i, \tilde{\beta}_i), (\tilde{\gamma}_i, \tilde{\delta}_i), 1 \leq i \leq \ell\}} \text{Res}(f_\pi, -\gamma_{(\eta_i, \epsilon_i)}) \epsilon_i,$$

where with $\gamma_{(a,b)} = \omega^2 a - \omega b$

$$f_\pi(k) := 3^\ell \omega^{m_\pi} \prod_{i=1}^\ell \frac{1}{(k + \gamma_{(\tilde{\alpha}_i, \tilde{\beta}_i)} + \mu)(k + \gamma_{(\tilde{\gamma}_i, \tilde{\delta}_i)} + \mu)}, \quad \mu := \omega^2 - \omega.$$

Proof. This is just a re-writing of formula of Theorem 4 in these rectangular coordinates. Indeed, the $(0, 0)$ -th entry of the matrix A_k^ℓ is, in these notation, equal to $\sum_{\pi \in \Theta_\ell} f_\pi(k)$. Because we work in a the Hilbert space $L^2(\mathbb{C}/\Gamma, \mathbb{C})$, this entry is also equal to $\langle A_k^\ell e_i, e_i \rangle_{L^2}$. Now, the poles of this function are exactly described by $\gamma_{(\tilde{\alpha}_i, \tilde{\beta}_i)} + \mu$ and $\gamma_{(\tilde{\gamma}_i, \tilde{\delta}_i)} + \mu$ (this is a consequence of formula A.1). Note however that in these coordinates, the poles get rescaled by $\sqrt{3}$, this is why $\mu = -i\sqrt{3}$ replaces $-i$. On the level of residues, this explains why a $\sqrt{3}$ does not appear in this formula. Finally, we remark that in this decomposition, $\gamma_{(\tilde{\alpha}_i, \tilde{\beta}_i)} + \mu \in \sqrt{3}(3\Gamma^* - i)$ and $\gamma_{(\tilde{\gamma}_i, \tilde{\delta}_i)} + \mu \in \sqrt{3}(3\Gamma^* - 2i)$ thus corresponding to the splitting appearing in the formula of stated in Theorem 4. \square

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Communicated by A.Giuliani