Integrability in the Chiral Model of Magic Angles

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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 \[ H(\alpha) = \begin{pmatrix} 0 & D(\alpha)^* \\ D(\alpha) & 0 \end{pmatrix} \] with \[ D(\alpha) = \begin{pmatrix} D_\bar{z} & \alpha U(z) \\ \alpha U(-z) & D_z \end{pmatrix} \]
where the parameter \( \alpha \) is proportional to the inverse relative twisting angle. After a simple rescaling, the potential is a smooth and periodic function satisfying
\[ U(z + a_\ell) = \bar{\omega}U(z), \quad U(\omega z) = \omega U(z), \quad \text{and} \quad U(\bar{z}) = \overline{U(z)}, \]
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
\[ U_0(z) = \sum_{k=0}^{2} \omega^k e^{\frac{1}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}. \]
Fig. 1. Plots of the first 5 non-negative eigenvalues of $H_{k}(0.3)$ acting on $\mathcal{H}$ (see (1.4) and (1.5)), as function of $k = (k_1\omega^2 - k_2\omega)/\sqrt{3}$ in in a fundamental cell of $3\Gamma^*$, parametrized by $(k_1, k_2) |k_j| < \frac{3}{2}$. 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

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

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

\[
H_k(\alpha) = \begin{pmatrix} 0 & D(\alpha)^* - \vec{k} \\ D(\alpha) - k & 0 \end{pmatrix}
\]

with \( k \in 3\Gamma^* \), \((1.4)\)
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

\[
\mathcal{H} := \{ v \in L^2(\mathbb{C}/\Gamma) : \mathcal{L}_a v = v, \ a \in \frac{1}{2} \Gamma \},
\]

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

\[
\text{Spec}_{L^2(\mathbb{C};\mathbb{C}^4)}(H(\alpha)) = \bigcup \text{Spec}_{\mathcal{H}}(H_k(\alpha)).
\]

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

\[
T_k = (2D_\bar{z} - k)^{-1} \begin{pmatrix} 0 & U(z) \\ U(-z) & 0 \end{pmatrix},
\]

then (see \([2, \text{Theorem 2}]\)) we have the following equivalence \([3, \S 2.3]\)

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

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 \( \alpha \) is inherently connected with the twisting angle, we shall refer to \( \alpha \)'s at which \((1.7)\) occurs as \textit{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 \( \alpha \) 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 eigenvalue.\(^2\) 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 \textit{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 \textit{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 \( \alpha, \mathcal{A} \subset \mathbb{C} \)—see Fig. 2.

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\(^1\) 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 $A$ of magic $\alpha$’s for which (1.7) holds, that is, the first band is flat. The positive elements of $A$ 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)

$$\text{tr}(T_{2\ell}^k) = \sum_{\alpha \in A} \alpha^{-2\ell} = \frac{\pi}{\sqrt{3}} q\ell \quad \text{with} \quad q\ell \in \mathbb{Q}. \quad (1.8)$$

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 $\alpha$’s, that is,

$$|A| = \infty.$$ 

This theorem will follow from the more general Theorem 6 and the observation that by the aforementioned explicit computation $\text{tr}_{\mathcal{H}}(T_4^k) = 8\pi/\sqrt{3}$ for $U = U_0$ there is at least one complex magic angle. We then focus on real magic angles. Since the operator $T_4^k$ is Hilbert–Schmidt, we can use the regularized determinant to study real magic $\alpha$. 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 \( \alpha \) satisfying \( |\alpha| < |\alpha_*| \), that is,

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

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 \( U(\bar{z}) = U(z) \) 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

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

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

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

if and only if

\[
u(z) = \sum_{n \in \mathbb{Z}^2} c_n e_{kn}
\]

where for \( n \in \mathbb{Z}^2 \)

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

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 \( \bar{u}(\bar{z}) = u(z) \) then

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

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

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

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

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

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

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

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

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)

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

$$L^2_{(p_1, p_2)} \xrightarrow{U(\pm z)} L^2_{(p_1 + 1, p_2 + 1)} \xrightarrow{(2D_{\bar{z}} - k)^{-1}} L^2_{(p_1 + 1, p_2 + 1)} \xrightarrow{U(z)} L^2_{(p_1, p_2)} \xrightarrow{(2D_{\bar{z}} - k)^{-1}} L^2_{(p_1, p_2)}.$$ This shows that we can restrict the operator $A_k$ to the subspaces $L^2_{(p_1, p_2)}$. From now on, we will denote by $A_k$ the restriction of $A_k$ to $L^2_{(1,1)}$. We then define the unitary multiplication operator

$$U_{(p_1, p_2)} : L^2_{(0,0)}(\mathbb{C}/\Gamma, \mathbb{C}^2) \to L^2_{(p_1, p_2)}(\mathbb{C}/\Gamma, \mathbb{C}^2),$$

$$U_{(p_1, p_2)}v(z) := e^{i(\bar{z}p_1 + \bar{z}p_2)}v(z), \quad p = \frac{1}{\sqrt{3}}(\bar{\omega}p_1 - \omega p_2), \quad p_j \in \mathbb{Z}_3,$$

$$U_{(p_1, p_2)}T_kU_{(p_1, p_2)^*} = T_{k-p}, \quad k \notin \Gamma^*.$$ The $k$-independence of the spectrum of $T_k$ implies then

$$\text{Spec}L^2_{(0,0)}(\mathbb{C}/\Gamma, \mathbb{C}^2)(T_k^2)\setminus\{0\} = \text{Spec}L^2_{(1,1)}(\mathbb{C}/\Gamma, \mathbb{C}^2)(T_k^2)\setminus\{0\} = \text{Spec}L^2_{(1,1)}(\mathbb{C}/\Gamma, \mathbb{C})(A_k)\setminus\{0\},$$ \quad (2.6)
where \( k \in D(0, r) \backslash \{0\} \), 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 \( D_\gamma^{-1} \) is defined on \( L^2_{(p, p)} \), \( p \neq 0 \mod 3 \). Since \( C \ni k \rightarrow A_k \mid_{L^2_{(1, 1)}} \) is an analytic family of operators with compact resolvents and the spectrum is independent of \( k \in \mathbb{C} \backslash 3\Gamma^* \), it follows that \( \text{Spec}(A_k) = \text{Spec}(A_0) \) [7, Theorem 1.10]. From (2.6) we obtain, as sets,

\[
\text{Spec}_{L^2_{(0, 0)}(T^2_p)} \{0\} = \text{Spec}_{L^2_{(1, 1)}(A_k)} \{0\}, \quad p \in D(0, r) \backslash \{0\}, \quad k \in D(0, r),
\]

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 \( \mathbb{C} \backslash ((3\Gamma^* - i) \cup (3\Gamma^* + i)) \). We conclude together with [3, Theorem 2] that

\[
\dim \ker_{\mathfrak{M}}(D(\alpha)) = \dim \ker_{L^2_{(1, 1)}}(A_0 - \alpha^{-2}).
\]

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 \( k \)
  \[
  \text{tr}(A_k^\ell) = \tau_\ell \text{ independent of } k \in \mathbb{C} \backslash (3\Gamma^* - i) \cup (3\Gamma^* + i).
  \]

- The function \( \mathbb{C} \backslash (3\Gamma^* - i) \cup (3\Gamma^* + i) \ni k \mapsto \langle A_k^\ell e_m, e_m \rangle_{L^2} \) is a finite sum of rational fractions on the complex plane \( \mathbb{C} \) with degree equal to \(-2\ell\) 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
  \[
  \langle A_k^\ell e_{3\gamma + i}, e_{3\gamma + i} \rangle_{L^2} = \langle A_{k - 3\gamma} e_i, e_i \rangle_{L^2}.
  \]

**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

\[
A_k^\ell e_{3\gamma + i} = \sum_{v \in F} R_{\nu + 3\gamma}(k) e_{\nu + 3\gamma},
\]

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

The result is clear for \( \ell = 0 \). Suppose the result true for \( \ell \), 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 \( e_v \) to a linear combination of \( e_{\ell} \) for \( \ell \in (3\Gamma^* + 2i) \). Then applying \( (D(0) - k)^{-1} \) multiplies the coefficient of \( e_{\ell} \) by \((\ell - k)^{-1}\). Multiplying by \( U(z) \) gives back a linear combination of \( e_v \) with \( v \in (3\Gamma^* + i) \). Finally, applying
\((D(0) - k)^{-1}\) multiplies the coefficient of \(e_v\) by \((v - k)^{-1}\). This means that, using the induction hypothesis (2.10),

\[
A_{\ell+1}^e e_{3^{\gamma+i}} = \sum_{\nu \in F} R_{\nu+3\gamma}(k) \sum_{\eta \in L} \sum_{\beta \in L} \frac{a_\eta}{k - (v + \beta - \eta + 3\gamma)} \frac{a_\beta}{k - (v + \beta + 3\gamma)} e_{\nu+\beta-\eta+3\gamma},
\]

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. \(\Box\)

### 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 \(k \not\in (3\Gamma^* - i) \cup (3\Gamma^* + i)\). We suppose that \(A_k\) satisfies the three properties stated in Lemma 2.2. Then one has, for any \(\ell \geq 2\),

\[
\tau_\ell = \frac{2i\pi \omega}{3\sqrt{3}} \sum_{\gamma \in \Gamma} n \left[ \sum_{m \in \mathbb{Z}} \text{Res}\left( \langle A_\ell^k e_i, e_i \rangle_{L^2}, \sqrt{3}(m\omega^2 - n\omega) + i \right) \right. 
\left. + \sum_{m \in \mathbb{Z}} \text{Res}\left( \langle A_\ell^k e_i, e_i \rangle_{L^2}, \sqrt{3}(m\omega^2 - n\omega) + 2i \right) \right],
\]

(3.1)

where all the infinite sums are in fact finite.

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

\[
k \in \mathbb{C}\backslash (3\Gamma^* - i) \cup (3\Gamma^* + i) \mapsto \langle A_\ell^k e_i, e_i \rangle_{L^2}.
\]

We first start by writing, using that \(A_\ell^k\) is trace-class for \(\ell \geq 2\),

\[
\tau_\ell = \sum_{\gamma \in \Gamma} \langle A_\ell^k e_{3^{\gamma+i}}, e_{3^{\gamma+i}} \rangle_{L^2}.
\]

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

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

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

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

The second property in Lemma 2.2 implies that

\[
\langle A_\ell^k e_i, e_i \rangle_{L^2} = O(k^{-2\ell}).
\]

(3.2)
Since we assume that \( \ell \geq 2 \), this justifies the exchange of integration and summation such that

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

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

\[
3 \tau_\ell = \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}} \langle A_{t+3n_1 \omega}^\ell, e_i \rangle_{L^2} dt.
\]

We now consider

\[
\int_{\mathbb{R}} \langle A_{t+3n_1 \omega}^\ell, e_i \rangle_{L^2} dt - \int_{\mathbb{R}} \langle A_{t+3(n+1)n_1 \omega}^\ell, e_i \rangle_{L^2} dt, \quad n \in \mathbb{Z}.
\]

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

\[
\int_{\mathbb{R}} \langle A_{t+3n_1 \omega}^\ell, e_i \rangle_{L^2} dt - \int_{\mathbb{R}} \langle A_{t+3(n+1)n_1 \omega}^\ell, e_i \rangle_{L^2} dt = 0.
\]

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

\[
3 \tau_\ell = \sum_{n \in \mathbb{Z}} n \left[ \int_{\mathbb{R}} \langle A_{t+3n_1 \omega}^\ell, e_i \rangle_{L^2} dt - \int_{\mathbb{R}} \langle A_{t+3(n+1)n_1 \omega}^\ell, e_i \rangle_{L^2} dt \right].
\]

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

\[
\int_{\Gamma_{n,R}} \langle A_{z}^\ell, e_i \rangle_{L^2} dz = \int_{\mathbb{R}} \langle A_{t+3n_1 \omega}^\ell, e_i \rangle_{L^2} \frac{\omega^2}{\sqrt{3}} dt - \int_{\mathbb{R}} \langle A_{t+3(n+1)n_1 \omega}^\ell, e_i \rangle_{L^2} \frac{\omega^2}{\sqrt{3}} dt.
\]

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

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

**Theorem 5.** Consider a potential \( U \in C^\infty (\mathbb{C} \setminus \Gamma; \mathbb{C}) \) 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 \( k \mapsto \langle A_{k}^{e_1}, e_1 \rangle_{L^2} \) is a rational fraction with coefficients in \( \mathbb{Q}(\omega/\sqrt{3}) \). This ring is actually a field as \( \omega/\sqrt{3} \) is algebraic over \( \mathbb{Q} \). Now, taking partial fraction expansion of \( k \mapsto \langle A_{k}^{e_1}, e_1 \rangle_{L^2} \) 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 \( k \mapsto \langle A_{k}^{e_1}, e_1 \rangle_{L^2} \) live in the field \( \mathbb{Q}(\omega/\sqrt{3}) \). But the uniqueness of the partial fraction expansion now gives that these are also the residues of \( k \mapsto \langle A_{k}^{e_1}, e_1 \rangle_{L^2} \) 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 \( \pi \) 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 \( i = 1, \ldots, N \) of \( A_{k}^{e_1} \). Then we define the \( n \)-th symmetric polynomial

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

Newton identities show that this polynomial can be expressed as

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

Newton identities show that this polynomial can be expressed as

\[
e_n(\lambda_1, \ldots, \lambda_N) = (-1)^n \sum_{m_1 + 2m_2 + \cdots + nm_n = n} \prod_{l=1}^{n} \frac{(-\text{tr} A_{k}^{2i_l})^{m_l}}{m_1!^{m_1}} \tag{3.6}
\]
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 \( m = (n, 0, \ldots, 0) \). The Newton identities for \( n > N \) then imply that the transcendental number \( \pi \) is a root of a polynomial with coefficients in \( \mathbb{Q} \left( \frac{\omega}{\sqrt{3}} \right) \). 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 \( a = (a_n)_{|n|\leq N} \in \mathbb{C}^{(2N+1)^2} \) 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 \( b = (b_n)_{|n|\leq N} \in \Omega_a \) we have \( \mathcal{A}(U_b) \neq \emptyset \). Take \( q = (q_n)_{|n|\leq N} \in (\mathbb{Q}(\omega/\sqrt{3}))^{(2N+1)^2} \cap \Omega_a \) 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 \( \Omega_a \). Hence, the set coefficients for which \( 0 < |A_b| < \infty \) is given by \( \bigcup_{m\in\mathbb{N}} \bigcup_{q\in\mathbb{Q}+i\mathbb{Q}} \Omega_q \setminus V_{m,q} \). 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

\[
\begin{align*}
D_k &:= \omega^2(D_{y_1} + k_1) - \omega(D_{y_2} + k_2), \\
V(y) &:= \sqrt{3}(e^{-i(y_1+y_2)} + \omega e^{i(2y_1-y_2)} + \omega^2 e^{i(-y_1+2y_2)}),
\end{align*}
\]

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

\[
\begin{align*}
\mathcal{D}_k^{-1} V_+ \mathcal{D}_k^{-1} V_- : L^2(\mathbb{C}/2\pi(\mathbb{Z} + i\mathbb{Z}) ) &\to L^2(\mathbb{C}/2\pi(\mathbb{Z} + i\mathbb{Z}) ) \quad \mathbb{C}.
\end{align*}
\]

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

\[
\begin{align*}
\hat{D}_k &:= \omega^2(D + k_1) - \omega(D + k_2), \quad \text{with } D = \text{diag}(\ell)_{\ell \in \mathbb{Z}} \\
\hat{V}_\pm(y) &:= \sqrt{3} \left( J_\pm \otimes J_\pm + \omega J_\mp \otimes J_\mp + \omega^2 J_\pm \otimes J_\mp \right),
\end{align*}
\]

(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)]
$$J^{p, q} \Lambda J^{p', q'} = \Lambda_{p, q} J^{p+p', q+q'} = J^{p+p', q+q'} \Lambda_{-p', -q'}.$$  
(4.3)
Denoting the inverse of $\hat{D}_k^{-1}$ by
$$\Lambda = \Lambda_k := \hat{D}_k^{-1}, \quad \Lambda_{m, n} = \frac{1}{\omega^2(m + k_1) - \omega(n + k_2)}, \quad (k_1, k_2) \notin \mathbb{Z}^2,$$
we see that $A_k$ reads in the new Fourier coordinates
$$\frac{1}{3} \hat{A}_k = \Lambda \Lambda_{1, 1} + \omega \Lambda \Lambda_{1, -2} + \omega^2 \Lambda \Lambda_{-2, 1} + \omega \Lambda \Lambda_{1, 1} J^{3, 0} + \omega \Lambda \Lambda_{1, 1} J^{0, 3}
+ \omega \Lambda \Lambda_{-2, 1} J^{-3, 0} + \omega^2 \Lambda \Lambda_{1, -2} J^{-3, 3} + \Lambda \Lambda_{1, -2} J^{3, -3}$$
with $\hat{A}_k$ the analogous restriction to $\ell^2_{(1, 1)}$.

4.2. Fredholm determinants. We start by defining the regularized Fredholm determinant
$$\det_2(1 - \alpha^2 \hat{A}_k) = \prod_{\lambda \in \text{Spec}(A_k)} E_1(\alpha^2 \lambda) \text{ with } E_1(z) = (1 - z)e^z \quad (4.4)$$
where the product respects multiplicities. We find from (2.6) that $\det_2(1 - \alpha^2 \hat{A}_k) = 0 \iff \alpha^{-1} \in \text{Spec}(T_k) \setminus \{0\}$. The symmetry of the spectrum of $\hat{A}_k$, $\text{Spec}(\hat{A}_k) = \text{Spec}(A_k)$, implies that $\alpha \mapsto \det_2(1 - \alpha^2 \hat{A}_k)$ 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 $C \ni \alpha \mapsto \det_2(1 - \alpha^2 \hat{A}_k)$ in (4.4) is an entire function, independent of $k \in \mathbb{C}$, which for any $n, m \in \mathbb{N}_0$ satisfies
$$\left| \frac{\partial^m_\alpha \det_2(1 - \alpha^2 \hat{A}_k) - \frac{\partial^m_\alpha}{\alpha^2} \sum_{j=0}^n \mu_j \frac{(-\alpha^2)^j}{j!} \right| \leq \sum_{j=n+1}^{\infty} \frac{\partial^m_\alpha}{\alpha^2} \left( \sqrt{\inf_{k \in \mathbb{C}} \| \hat{A}_k \|_2 |\alpha|^2} \right)^j$$
with $\|A_0\|_2 \leq 2$, where
$$\mu_j := \det \begin{pmatrix} 0 & j - 1 & 0 & \cdots & 0 \\ \sigma_2 & 0 & j - 2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \sigma_{j-1} & \sigma_{j-2} & \cdots & 0 & 1 \\ \sigma_j & \sigma_{j-2} & \cdots & 0 & 0 \end{pmatrix}, \quad \text{with } \sigma_j = \text{tr} \hat{A}_k^j. \quad (4.5)$$
Proof. The expression (4.4) is well-defined since \( \hat{A}_k \) is a Hilbert-Schmidt operator and the Taylor coefficients \( \mu_j \) are for example stated in [8, (6.13)]. Indeed, since \( |E_1| \leq e^{\frac{|z|^2}{2}} \) for \( z \in \mathbb{C} \) and \( \sum_{\lambda \in \text{Spec}(\hat{A}_k)} |\lambda|^2 \leq \| \hat{A}_k \|^2_2 \), we conclude that

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

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

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

which is optimized at \( |\alpha|^2 = \frac{\sqrt{7}}{\| \hat{A}_k \|^2_2} \), such that

\[
|\mu_j| \leq \frac{\| \hat{A}_k \|^j_2 e^{j/2} j!}{j^{j/2}}.
\]

The Taylor coefficients \( \mu_j \) are then given by the Plemelj-Smithies formula [8] stated in (4.5). Since they only depend on traces \( \sigma_j \) 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 \( \hat{A}_0 = (\hat{A}_0(n))_{n \in \mathbb{Z}^2} \) and let \( P_m \) be the projection onto \( (3\{-m, -m + 1, ..., m\} + 1)^2 \), then

\[
\| \hat{A}_0 \|^2_2 \leq \| P_M \hat{A}_0 \|^2_2 + \| (\text{id} - P_M) \hat{A}_0 \|^2_2. \tag{4.7}
\]

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

\[
\| P_M \hat{A}_0 \|^2_2 = \sqrt{\text{tr}(P_M \hat{A}_0 \hat{A}_0^* P_M)} \leq 5 \text{ for } M = 760.
\]

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

\[
\| (\text{id} - P_M) \hat{A}_0 \|^2_2 \leq 9 \| (\text{id} - P_M)(\mathcal{D}_0^{-1})_{\ell^2_2 \rightarrow \ell^2_{(2,2)}} \|_4 \| (\mathcal{D}_0^{-1})_{\ell^2_2 \rightarrow \ell^2_{(2,2)}} \|_4. \tag{4.8}
\]

We recall that by definition

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

A simple change of variables shows that \( \| (\mathcal{D}_0^{-1})_{\ell^2_{(1,1)} \rightarrow \ell^2_{(1,1)}} \|_4 = \| (\mathcal{D}_0^{-1})_{\ell^2_{(2,2)} \rightarrow \ell^2_{(2,2)}} \|_4. \)

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

While an explicit computation shows using exact symbolic calculations
\[ \sum_{|m| \leq 6} \frac{1}{g(m)^2} \leq \frac{24}{7} \] \hspace{1cm} (4.9)

Then, we may use for \(|m|\) > 6 that \( g(m) \geq |m|^2 + 5^2 \), such that we can estimate the remainder
\[ \sum_{|m| \geq 7} \frac{1}{g(m)^2} \leq \frac{\pi}{61} \] \hspace{1cm} (4.10)

Inserting this estimate into (4.8), we find along the lines of (4.10)
\[ \| (\mathcal{D}^{-1}_0) \ell^2_{(2,2)} \to \ell^2_{(2,2)} \|_4 \leq \left( \frac{8}{21} + \frac{\pi}{549} \right)^{1/4}. \]

which shows that \( \| \hat{A}_0 \|_2 < \frac{11}{12} \).

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 \( \frac{1}{\alpha^2} \) to the operator \( \hat{A}_k \), independent of \( k \in \mathbb{C} \), with \( \alpha \in (0.583, 0.589) \) such that \( \frac{1}{\alpha^2}, \infty \subset \mathbb{R} \setminus \text{Spec}(\hat{A}_k) \).

**Proof.** To see that this is the first real magic angle, we first notice that the operator norm
of \( \hat{A}_0 \) is bounded by
\[ \| \hat{A}_0 \| \leq (3\sqrt{3})^2 \| (\mathcal{D}_0^{-1}) \ell^2_{(1,1)} \to \ell^2_{(1,1)} \|^2 = 9. \]

This estimate shows that \( \alpha \in \mathbb{R}^+ \) with \( 1/(\alpha^2) \) \( \in \text{Spec}(\hat{A}_0) \) 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
\[ r_i \leq \left( \frac{2\nu}{\alpha} \right)^i \left( \frac{\nu}{\sqrt{N}} \right)^{N-i} \text{ for } r_0 := \sum_{k=N}^{\infty} \left( \frac{\nu}{\sqrt{k}} \right)^k \text{ and } r_1 := \sum_{k=N}^{\infty} \frac{2k}{\alpha} \left( \frac{\nu}{\sqrt{k}} \right)^k. \]
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Table 1. First eight exact traces of $A_k^p$, $\sigma_p = \text{tr}(A_k^p)$, with floating point approximation, where $\sigma_1 := \lim_{n \to \infty} \sum_{|i| \leq n} \langle A_k e_i, e_i \rangle$ 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 $\sigma_2/\sigma_1 \approx 1/0.5857^2 = 2.91507$, for $p$ large, where 0.5857 is the first magic angle

| $p$ | $\frac{\sigma_p \sqrt{3}}{\pi}$ |
|-----|---------------------------------|
| 1   | $\frac{2}{3}$                  |
| 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 $\nu = \sqrt{e\|\hat{A}_0\|_2}2\alpha^2$, as in the error bound stated in Lemma 4.1, with upper bound $\|\hat{A}_0\|_2 = 5.5$, we obtain for $\alpha = \frac{3}{5}$ that $r_0 \leq \frac{1}{30}$ 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

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

One then checks (using computations involving integers only)

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

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

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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 $A^\ell_k$ is of the form

$$(A^\ell_k)_{ii} = 3^\ell \sum_{\pi \in \Theta^\ell} \omega^{m\pi} \prod_{i=1}^\ell \Lambda_{\tilde{\alpha}_i, \tilde{\beta}_i} \Lambda_{\tilde{\gamma}_i, \tilde{\delta}_i},$$

(A.1)

where

$$\tilde{\alpha}_i = \sum_{j=1}^{i-1} \alpha_j + \gamma_j, \quad \tilde{\beta}_i = \sum_{j=1}^{i-1} \beta_j + \delta_j, \quad \tilde{\gamma}_i = \alpha_i + \sum_{j=1}^{i-1} \alpha_j + \gamma_j,$$

$$\tilde{\delta}_i = \beta_i + \sum_{j=1}^{i-1} \beta_j + \delta_j, \quad m_{\pi} := \frac{2}{3} \sum_{i=1}^\ell (\gamma_i + \beta_i).$$

(A.2)

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

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

Using (A.1), the diagonal part of $A^\ell_k$, is of the form

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

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

$$\Lambda'_{m,n} = \frac{1}{\omega^2(3m + 1 + k_1) - \omega(3n + 1 + k_2)}.$$
Theorem 7. Let $\ell \geq 2$ and $\Theta_\ell$ be as in (A.3) with coefficients $\tilde{a}_i, \ldots, \tilde{d}_i, m_\pi$ as in (A.2). Then the traces are given by

$$\text{tr} \left( A^\ell_k \right) = -\frac{2i\omega\pi}{3} \sum_{\pi \in \Theta_\ell} \sum_{(\eta_i, \epsilon_i) \in \{ (\tilde{a}_i, \tilde{b}_i), (\tilde{c}_i, \tilde{d}_i), 1 \leq i \leq \ell \}} \text{Res}(f_\pi, -\gamma(\eta_i, \epsilon_i)) \epsilon_i,$$

where with $\gamma(a, b) = \omega^2 a - \omega b$

$$f_\pi(k) := 3^\ell \omega^m \pi \prod_{i=1}^\ell \frac{1}{(k + \gamma(\tilde{a}_i, \tilde{b}_i) + \mu)(k + \gamma(\tilde{c}_i, \tilde{d}_i) + \mu)}, \quad \mu := \omega^2 - \omega.$$

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 $A^\ell_k$ 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 $(A^\ell_k e_i, e_i)_{L^2}$. Now, the poles of this function are exactly described by $\gamma(\tilde{a}_i, \tilde{b}_i) + \mu$ and $\gamma(\tilde{c}_i, \tilde{d}_i) + \mu$ (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, $\gamma(\tilde{a}_i, \tilde{b}_i) + \mu \in \sqrt{3}(3\Gamma^* - i)$ and $\gamma(\tilde{c}_i, \tilde{d}_i) + \mu \in \sqrt{3}(3\Gamma^* - 2i)$ thus corresponding to the splitting appearing in the formula of stated in Theorem 4. □

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