

# RAPPORT DE STAGE M1

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## 1. DÉBUT DU STAGE ET INTRODUCTION AU PROBLÈME.

1.1. **Commentaires sur le stage.** Le stage s'est déroulé du 1 février au 31 mai 2022, soit exactement 4 mois à Berkeley sous la direction de Maciej Zworski. Maciej est un expert de l'analyse semi-classique, domaine que j'ai découvert au premier semestre en

suis des cours du M2 de Jussieu et que je pense continuer l'année prochaine.

Pendant le premier confinement, il a été contacté pour participer à un projet de mathématiques appliquées à la physique de la matière condensée. Les mathématiques utilisées sont relativement élémentaires et les opérateurs en jeu exhibent un comportement spectral très étrange. Il m'a proposé de travailler sur ce projet, voulant essentiellement être confronté à la recherche pendant ces 4 mois, j'ai accepté.

J'ai énormément apprécié la liberté et l'autonomie que l'on m'a donné. J'ai suivi un seul cours (de systèmes dynamiques) et j'ai utilisé le reste du temps libre pour suivre les divers séminaires du département de math. La plus grande part de mes journées consistait à faire de la recherche, ce qui est une bonne situation étant donné le cadre de vie à Berkeley. J'ai eu l'occasion de rencontrer de bons amis et j'ai pu participer à de nombreux séminaires dont l'un à Stanford et l'un à UCLA. Je souhaite remercier particulièrement Maciej pour le temps qu'il a pris pour s'occuper de moi ainsi que pour la confiance qu'il a placée en moi. Ce stage a été un excellent premier contact avec le monde de la recherche et a, sur beaucoup de points, changé ma perception de ce dernier, pour le meilleur.

**1.2. Introduction au problème.** Une expérience réalisée au MIT en 2019 par Tarnopolsky, Kruchkov et Vishwanath a montré que lorsque deux plaques de graphène (penser à un réseau hexagonal) sont posées l'une sur l'autre, rotatée l'une par rapport à l'autre d'un certain angle  $\theta$  précis, on observe de la supraconductivité. Ces angles ont été nommés "angles magiques" et sont l'objet d'étude de ce projet.

Mathématiquement, le problème est modélisé par l'hamiltonien de Bistritzer-MacDonald défini comme suit:

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

Ici,  $U$  est un potentiel modélisant les interactions entre les plaques de graphène. Le paramètre  $\alpha$  est essentiellement l'inverse de l'angle entre les deux plaques. Le graphène a une structure de réseau hexagonal, cela se traduit sur le potentiel  $U$  par les symétries suivantes:

$$U(z + \mathbf{a}_i) = \bar{\omega}U(z), \quad U(\omega z) = \omega U(z), \quad \text{et } U(\bar{z}) = \overline{U(z)}, \quad (1.1)$$

où  $\omega = e^{2\pi i/3}$  et  $\mathbf{a}_i = \frac{4}{3}\pi i \omega^i$ . L'exemple le plus simple de tel potentiel est donné par  $U_0(z) = \sum_{k=0}^2 \omega^k e^{\frac{1}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}$ . Le hamiltonien  $H(\alpha)$  est un opérateur qui agit sur l'espace de Hilbert  $H^1(\mathbb{C}/\Gamma; \mathbb{C}^4)$  et  $D(\alpha)$  sur l'espace  $H^1(\mathbb{C}/\Gamma; \mathbb{C}^2)$ , où on a noté  $\Gamma = 4\pi i(\mathbb{Z} + \omega\mathbb{Z})$  le réseau hexagonal formé par la superposition des deux plaques de graphène (on parle d'effet Moiré). Les propriétés physiques surprenantes mises en évidence par l'expérience se traduisent en propriétés spectrales tout aussi étonnantes sur ces opérateurs.

1.2.1. *Le problème mathématique.* Dans un article publié en 2021, Zworski, Becker, Embree et Wittsen, ont donné plusieurs caractérisations spectrales des angles magiques. Commençons par une définition.

On dit que  $\alpha \in \mathbb{C}$  est un angle magique si et seulement si

$$\text{Spec}_{H^1(\mathbb{C}/\Gamma)} D(\alpha) = \mathbb{C}.$$

On notera  $\mathcal{A}$  l'ensemble des angles magiques (complexes).

**Remark 1.** *Il ne s'agit pas de la définition physique mais elle est équivalente et c'est celle-ci que l'on utilisera.*

Dans l'article, ils montrent notamment que l'on observe le comportement spectral suivant très étonnant.

**Theorem 1.** *L'application  $\alpha \in \mathbb{C} \mapsto D(\alpha)$  est analytique, l'opérateur  $D(\alpha)$  est elliptique, de Fredholm d'indice 0 et on a*

$$\begin{cases} \text{Spec}_{H^1(\mathbb{C}/\Gamma)} D(\alpha) = \mathbb{C} & \text{si } \alpha \in \mathcal{A} \\ \text{Spec}_{H^1(\mathbb{C}/\Gamma)} D(\alpha) = \Gamma^* & \text{sinon.} \end{cases}$$

Où  $\Gamma^* = \frac{1}{\sqrt{3}} (\mathbb{Z} + \omega\mathbb{Z})$  est le réseau dual de  $\Gamma$ .

**Remark 2.** *Il y a un peu de vocabulaire de théorie spectrale mais on peut reformuler le théorème comme suit:*

*"La famille d'opérateurs  $D(\alpha)$  est analytique (en quelque sorte la plus régulière possible) et a de "bonnes" propriétés spectrales (penser à  $D(\alpha)$  comme une matrice infinie), mais son spectre varie de façon discontinue. Le spectre est discret et constant sur la plupart du domaine et à certains points précis (qui sont les angles magiques) il vaut tout le plan complexe."*

Il est bon de noter que ce n'est pas le tout premier exemple de telle famille d'opérateurs (on a notamment un exemple donné par Seyley auparavant) mais que cela donne une motivation physique à ce phénomène. De plus, le théorème précédent est valide pour tout choix de potentiel  $U$  ayant les symétries énoncées au début et produit donc une famille infinie d'exemples.

Cette définition des angles magique n'est pas facile à appréhender mathématiquement (et il est difficile de calculer ces angles magiques même numériquement). En effet, il est difficile de vérifier que le spectre de  $D(\alpha)$  soit égal à tout le plan complexe. Toujours dans le même papier, ils énoncent et démontrent le théorème suivant qui donne une caractérisation plus simple des angles magiques:

**Theorem 2.** *Pour  $k \notin \Gamma^*$ , définissons l'opérateur compact (dit de Birman-Schwinger)*

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

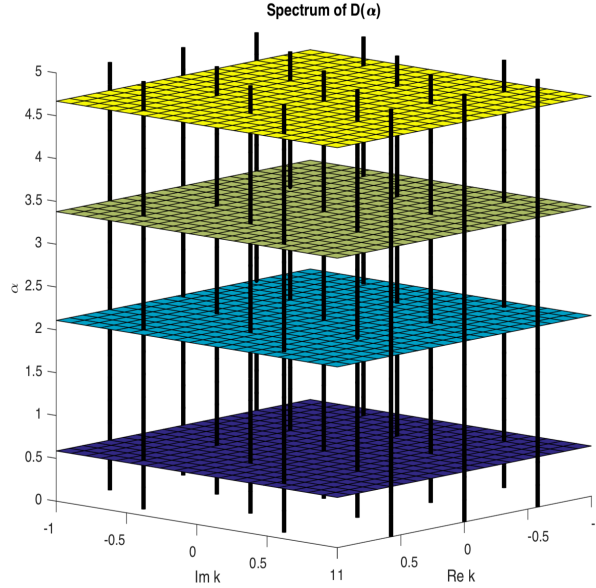


FIGURE 1. Graphe du spectre de  $D(\alpha)$  pour  $\alpha \in \mathbb{R}$ . On voit que le spectre est constant égal à  $\Gamma^*$  sauf pour certaines valeurs de  $\alpha$ . Ces derniers sont les angles magiques, points où la discontinuité se produit.

Alors on a l'équivalence suivante:

$$\alpha \in \mathcal{A} \iff \frac{1}{\alpha} \in \frac{1}{\text{Spec}_{L^2(\mathbb{C}/\Gamma)}(T_k) - \{0\}}.$$

En particulier, le spectre de  $T_k$  ne dépend pas de  $k \notin \Gamma^*$ .

**Remark 3.** On se ramène donc à calculer le spectre d'un opérateur compact (penser à une matrice infinie). La structure est toujours la même, à chaque équivalence, on simplifie la condition spectrale mais l'opérateur devient un peu moins facile à appréhender. Remarquons que l'opérateur  $H(\alpha)$  était autoadjoint et que  $T_k$  n'est même plus normal. Il s'agit de la principale raison pour laquelle l'étude spectrale de  $T_k$  n'est pas évidente. (Penser à comment les blocs de Jordan sont la principale difficulté à surmonter pour l'étude spectrale des matrices non diagonalisables).

**1.3. Généralisation à d'autres groupes.** L'équivalence spectrale plus haut repose sur deux éléments: les propriétés du groupe de symétries du graphène (qui est un réseau hexagonal) et les propriétés spectrales de l'opérateur  $D(0) = D_{\bar{z}}$ .

Le groupe des isométrie du réseau hexagonal est  $p3$ , l'un des 17 groupes cristallographiques. La première idée était donc de voir si l'on pouvait utiliser les autres groupes cristallographiques pour construire d'autre familles d'opérateurs comme  $D(\alpha)$ . Il s'agit essentiellement d'étudier les représentations irréductibles de certains produits semi-directs de groupes cristallographiques par des groupes abéliens. J'ai appris pas

mal de choses mais malheureusement, je n'ai pas réussi à généraliser aux autres groupes. La seule extension (triviale) est au groupe  $p2$ , groupe de symétries du réseau carré. Toutefois, pour le réseau carré, les angles magiques générés (numériquement) ne semblent jamais être réels. Il s'agit donc d'un exemple moins intéressant pour les physiciens même si on ne sait toujours pas pourquoi c'est le cas.

## 2. TRACES ET PRINCIPAL RÉSULTAT.

**2.1. Rationalité et infinité d'angles magiques.** Un problème (passé sous le tapis jusqu'ici) est le fait que l'on a pas prouvé que  $\mathcal{A} \neq \emptyset$ . En effet, il est a priori tout à fait possible que le spectre de  $T_k$  soit réduit à  $\{0\}$  (on parle d'opérateur quasi-nilpotent, remarquons tout de même que pour un opérateur normal non nul, c'est impossible).

Les hypothèses que l'on dispose sur  $T_k$  sont essentiellement calculatoires. On peut notamment définir les traces de puissances de  $T_k$ . Toujours dans le même article, ils calculent que pour le potentiel  $U_0$ , on a  $\text{Tr}(T_k^4) = \sum_{\alpha \in \mathcal{A}} \alpha^{-4} = \frac{8\pi}{\sqrt{3}} \neq 0$ . Le calcul est assez miraculeux et peu éclairant mais montre que  $\mathcal{A} \neq \emptyset$ . De manière générale, il n'est pas très difficile de calculer (numériquement) le spectre de  $T_k$  (car ce dernier est très bien approximé par le spectre de matrices finies). On remarque un grand nombre de structures dans le spectre. Toutefois, tout ceci est très dur à montrer mathématiquement. Il y a notamment deux problèmes importants: on ne sait pas montrer l'existence d'angles magiques réels (qui semblent toujours exister numériquement et qui sont les angles physiquement pertinents) ni montrer que les angles magiques sont en nombre infini. Numériquement, il semble aussi que la valeur de  $\text{Tr}(T_k^{2l})$  soit toujours de la forme  $q_l \frac{\pi}{\sqrt{3}}$  pour  $q_l \in \mathbb{Q}$ , c'est la question à laquelle Maciej m'a demandé de réfléchir à partir du second mois de stage.

Il s'agit de ma principale contribution pendant ce stage. Je suis parvenu à montrer la conjecture en donnant une manière algorithmique de calculer ces traces (remarquons que cet algorithme peut être adapté pour calculer les traces d'autres opérateurs définis pour des potentiels  $U$  généraux).

**Theorem 3.** *Pour  $l \geq 2$ ,*

$$\text{Tr}(T_k^{2l}) = \sum_{\alpha \text{ magic}} \alpha^{-2l} = q_l \frac{\pi}{\sqrt{3}} \text{ où } q_l \in \mathbb{Q}.$$

On en déduit d'ailleurs l'amélioration du résultat précédent.

**Corollary 2.1.** *Pour  $U = U_0$ , l'ensemble des angles magiques  $\mathcal{A}$  est infini.*

On en déduit aussi par un argument similaire que le corollaire précédent est valable pour un ensemble générique (au sens de Baire) de potentiels. Cela répond donc (partiellement) au second problème. En effet, pour un potentiel  $U$  quelconque, il existe donc des perturbations arbitrairement proches de  $U$  admettant une infinité d'angles

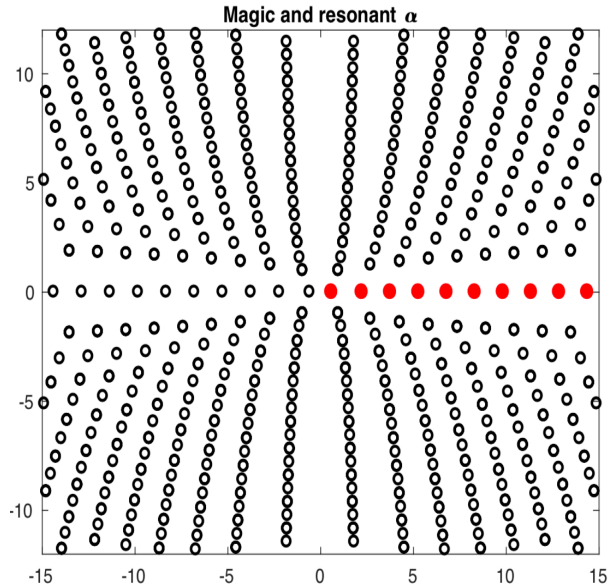


FIGURE 2. Ensemble des angles magiques générés numériquement grâce à l’opérateur  $T_k$ . Les  $\alpha$  rouges sont les angles physiquement pertinents.

magiques.

Les techniques utilisées sont relativement élémentaires: un peu de combinatoire, d’analyse complexe sur les courbes elliptiques et beaucoup de courage. Cela m’a occupé un mois et demi. Il se trouve que ce calcul peut permettre de répondre (partiellement) au premier problème soulevé. Il s’agit d’une remarque faite par Simon Becker avec qui j’ai collaboré pendant la seconde moitié du stage.

**2.2. Déterminant et angle magique réel.** L’argument précédent peut sembler étrange, pourquoi calcule t’on les traces? La réponse pragmatique est que l’on ne sait pas calculer grand chose d’autre. Il se trouve néanmoins qu’il y a une justification plus profonde: la fonction déterminant.

Pour un opérateur  $A$  trace class (c’est à dire un opérateur compact dont la suite des valeurs singulières  $(\mu_i(A))_{i \in \mathbb{N}}$ , i.e la suite des racines carrées des valeurs propres de  $AA^*$ , est sommable), on définit la fonction déterminant par

$$\det(I_d + \mu A) := \prod_{i \in \mathbb{N}} (1 + \mu \lambda_i(A)) = \exp(\text{Tr}(\ln(I_d + \mu A))).$$

Cela définit une fonction entière qui s’annule exactement en les  $\lambda_i(A)$  (et avec la bonne multiplicité) et cette dernière caractérise donc entièrement le spectre. Il faut penser à cette fonction comme une généralisation ”naturelle” du polynôme de Cayley-Hamilton pour une matrice infinie (l’hypothèse de sommabilité étant nécessaire pour s’assurer que la définition est bien posée). En particulier, il existe des formules (dites de Plemelj

et Smithies) qui permettent de calculer les coefficients de la fonction de déterminant en fonction des traces des puissances de  $A$ . (Encore une fois, cela est une généralisation de ce qui se passe pour les matrices). Essentiellement, connaître les traces des  $n$  premières puissances de  $A$  donne les  $n$  premiers coefficients de la fonction déterminant. Ainsi, la connaissance de toutes les traces équivaut à la connaissance du spectre. Dans notre cas, notre opérateur n'est pas trace class ( $(\mu_i(A))_{i \in \mathbb{N}}$  n'est pas  $l^1$  mais  $l^4$ ), toutefois, on peut définir un déterminant dit "régularisé" et les mêmes conclusions tiennent. Nous avons implémenté l'algorithme pour calculer les 6 premières traces et par des arguments directs, nous avons montré l'existence d'un angle magique réel. Nous avons aussi montré que la multiplicité de cet angle était 1.

**Theorem 4.** *Le hamiltonnien  $H(\alpha)$  admet un angle magique de multiplicité 2 tel que  $\alpha_* \in (0.583, 0.589)$ . En particulier,  $\alpha_*$  est minimal, c'est à dire qu'il n'existe pas d'autres angles magiques  $\alpha$  tels que  $|\alpha| < |\alpha_*|$ .*

**Remark 4.** *Il s'agit d'une preuve assistée par ordinateur (notamment pour calculer les valeurs des traces). Ce n'est pas la première preuve (assistée par ordinateur) du fait qu'un angle magique réel existe mais celle-ci fournit en plus la simplicité de la valeur propre qui a été très importante pour la fin de ce stage.*

Enfin, tout ceci a donné lieu à un article co-écrit avec Simon Becker et Maciej Zworski dont le pré-print a été réjouté ci-dessous.

### 3. FIN DU STAGE

Le dernier mois a été plus tranquille. J'ai notamment eu l'occasion d'aller en séminaire à Stanford ainsi qu'à UCLA pour un séminaire de 5 jours sur la physique de la matière condensée. Ce fût une bonne expérience même si les séminaires étaient assez durs à comprendre pour un matheux comme moi.

Maciej m'a fait travailler sur un second article, ma contribution cette fois-ci est essentiellement technique et il s'agit d'étudier le nombre de zéros des fonctions propres du hamiltonnien (c'est un résultat qui s'appuie sur la simplicité de l'angle magique prouvé plus haut). Ce travail (sur lequel je continue de travailler pendant l'été) va normalement aussi aboutir à un article.

### 4. CONCLUSION

C'était un stage très chouette.

## 5. PRE-PRINT.

# Integrability in chiral model of magic angles

ABSTRACT. Magic angles in the chiral model of twisted bilayer graphene are characterized in terms of a dimensionless parameter  $\alpha \in \mathbb{C}$  which (for  $\alpha$  real) is inversely proportional to the twisting angle and at which the Hamiltonian exhibits a flat band at energy zero. We show that for any  $\ell \geq 2$ , the sum over *magical* (complex)  $\alpha$ 's satisfies  $(\sqrt{3}/\pi) \sum \alpha^{-2\ell} \in \mathbb{Q}$  and that this value is algorithmically computable. This implies that the set of *magical*  $\alpha$ 's is infinite and provides a new proof of the existence of the first real magic angle, showing also that the corresponding flat band has minimal multiplicity.

## 6. 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 [BiMa11, CGG22]

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

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

$$U(z + \mathbf{a}_\ell) = \bar{\omega}U(z), \quad U(\omega z) = \omega U(z), \text{ and } U(\bar{z}) = \overline{U(z)}, \quad (6.1)$$

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

$$U(z) = \sum_{k=0}^2 \omega^k e^{\frac{1}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}. \quad (6.2)$$

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

$$\mathcal{L}_{\mathbf{a}} \mathbf{w}(z) := \begin{pmatrix} \omega^{a_1+a_2} & 0 \\ 0 & 1 \end{pmatrix} \mathbf{w}(z + \mathbf{a}), \quad \mathbf{a} \in \frac{1}{3}\Gamma, \quad (6.3)$$

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

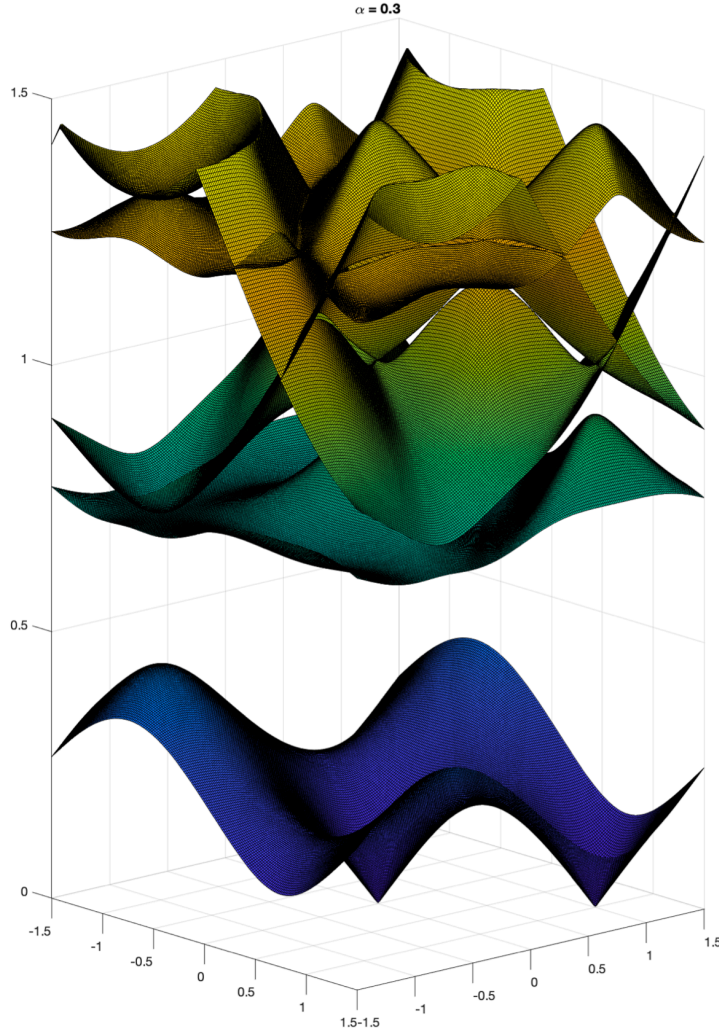


FIGURE 3. Plots of the first 5 non-negative eigenvalues of  $H_{\mathbf{k}}(0.3)$  acting on  $\mathcal{H}$  (see (6.4) and (6.5)), as function of  $k = (k_1\omega^2 - k_2\omega)/\sqrt{3}$  in a fundamental cell of  $3\Gamma^*$ , parametrized by  $(k_1, k_2)$   $|k_j| < \frac{3}{2}$ . See also [BHZ22, Figure 4] for more information and comparison with band structure of other models.

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  $\mathcal{L}_{\mathbf{a}}$  to an action on each  $\mathbb{C}^2$  component. We then consider the Floquet spectrum of

$$H_{\mathbf{k}}(\alpha) = \begin{pmatrix} 0 & D(\alpha)^* - \bar{k} \\ D(\alpha) - k & 0 \end{pmatrix} \text{ with } k \in 3\Gamma^*, \quad (6.4)$$

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

$$\mathcal{H} := \{\mathbf{v} \in L^2(\mathbb{C}/\Gamma) : \mathcal{L}_{\mathbf{a}}\mathbf{v} = \mathbf{v}, \quad \mathbf{a} \in \frac{1}{3}\Gamma\}, \quad (6.5)$$

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. The appearance of perfectly flat bands in the chiral limit was considered by San–Jose, González and Guinea [SGG12] and was explained by Tarnopolsky, Kruchkov and Vishwanath [TKV19] with the help of Jacobi theta functions<sup>1</sup>. An equivalent spectral theoretic characterization of magic angles was then provided in [Be\*22]: if we define the following compact Birman-Schwinger operator

$$T_k = (2D_{\bar{z}} - k)^{-1} \begin{pmatrix} 0 & U(z) \\ U(-z) & 0 \end{pmatrix}. \quad (6.6)$$

then (see [Be\*22, Theorem 2] and for a more general version stated here [BHZ22, §2.5])

$$0 \in \bigcap_{k \in \mathbb{C}} \text{Spec}_{\mathcal{H}}(H_k(\alpha)) \iff \begin{cases} \alpha^{-1} \in \text{Spec}_{\mathcal{H}}(T_{k_0}) \\ \text{for some } k_0 \in \mathbb{C} \setminus (3\Gamma^* - \{0, i\}), \end{cases} \quad (6.7)$$

where  $\mathcal{H}$ . 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 (6.7) 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  $\alpha$  at which the Hamiltonian exhibits a flat band at zero energy is non-trivial. In [Be\*22] the existence of such a complex parameter  $\alpha \in \mathbb{C}$  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<sup>2</sup>. This result was improved by a computer-assisted proof [WaLu21] in which Watson and Luskin used the complex-analytic characterization of magic angles from [TKV19] to prove existence of the first *real* magic angle and obtained explicit bounds on its position.

In this article, we obtain a general result about the structure of the traces of powers of  $T_k$ . It seems to reflect hidden *integrability* properties of the Hamiltonian  $H(\alpha)$  for

<sup>1</sup>As was pointed out to us by Alex Sobolev a similar argument appeared in the work of Dubrovin and Novikov [DuNo80] who studied magnetic Hamiltonians on tori.

<sup>2</sup>In [Be\*22] we considered the trace on  $L^2(\mathbb{C}/\Gamma; \mathbb{C}^2)$  which gave this answer multiplied by 9 – see [BHZ22, §2.4].

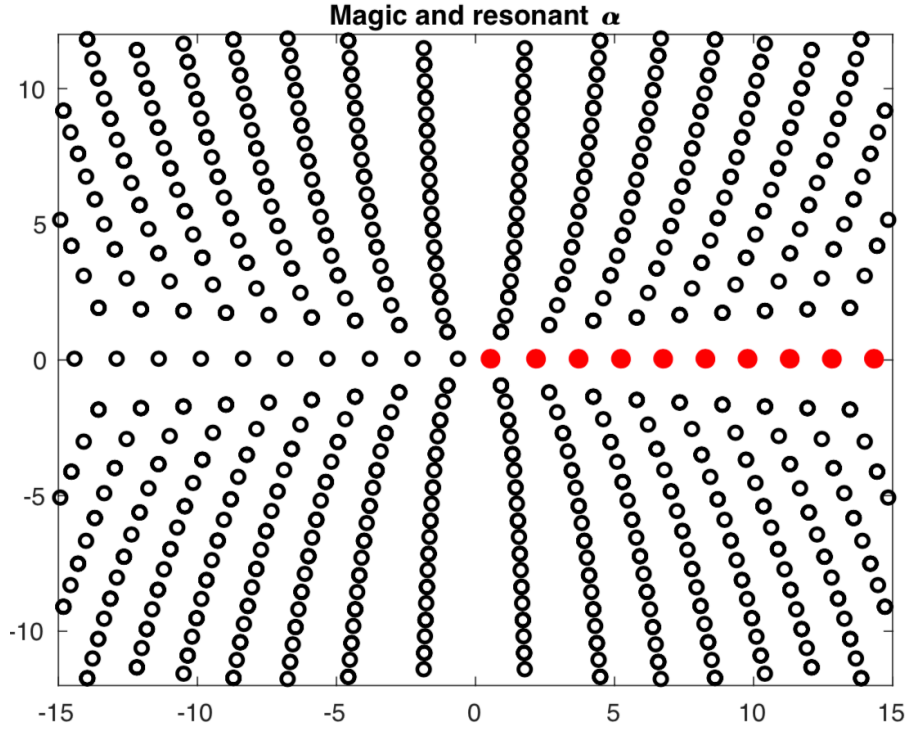


FIGURE 4. The set  $\mathcal{A}$  of magic  $\alpha$ 's for which (6.7) holds, that is, the first band is flat. The positive elements of  $\mathcal{A}$  are the reciprocals of the “physically relevant” positive angles. Potential (6.2) is responsible for the regularity of the set which seems to indicate 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 (6.1). The animation also indicates changing multiplicities.

the potential (6.2). These are already visible in the regular but evasive structure of the set of of magic  $\alpha$ ,  $\mathcal{A} \subset \mathbb{C}$  – see Figure 4.

**Theorem 5.** For  $\ell \geq 2$

$$\text{tr}(T_k^{2\ell}) = \sum_{\alpha \in \mathcal{A}} \alpha^{-2\ell} = \frac{\pi}{\sqrt{3}} q_\ell \quad \text{with } q_\ell \in \mathbb{Q}. \quad (6.8)$$

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 8. As we show in §9, it is already possible to conclude directly from Theorem 5 that

**Theorem 6.** *There exist infinitely many magic  $\alpha$ 's, that is,*

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

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  $\alpha$ . Compared with the initial approach proposed in [TKV19], this approach has two advantages. Unlike the series expansion in [TKV19, WaLu21], 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 5. This leads to

**Theorem 7.** *The chiral Hamiltonian 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,*

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

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

**Remark.** Compared with results in [WaLu21] 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.

## 7. PRELIMINARIES

Here we recall some facts from [Be\*22] and [BHZ22] needed in this paper. For most of our analysis, it is convenient to use rectangular coordinates  $z = 2i(\omega y_1 + \omega y_2)$ , see [Be\*22, §3.3] for details. In these coordinates, we may introduce

$$\begin{aligned} \mathcal{D}_k &:= \omega^2(D_{y_1} + k_1) - \omega(D_{y_2} + k_2), \\ \mathcal{V}(y) &:= \sqrt{3}(e^{-i(y_1+y_2)} + \omega e^{i(2y_1-y_2)} + \omega^2 e^{i(-y_1+2y_2)}), \end{aligned} \tag{7.1}$$

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 Birman-Schwinger operator  $T_k$ , with  $k = (\omega^2 k_1 - \omega k_2)/\sqrt{3}$ ,  $(k_1, k_2) \notin 3\mathbb{Z}^2 + \{(0, 0), (-1, -1)\}$  (we remark that  $\mathbb{Z}^2$  corresponds to  $\Gamma^*$  – see [BHZ22, (2.12)]) is then given by

$$T_k := \begin{pmatrix} 0 & \mathcal{D}_k^{-1} \mathcal{V}_+ \\ \mathcal{D}_k^{-1} \mathcal{V}_- & 0 \end{pmatrix} : L_{(0,0)}^2(\mathbb{C}/2\pi\mathbb{Z}^2; \mathbb{C}^2) \rightarrow (H^1 \cap L_{(0,0)}^2)(\mathbb{C}/2\pi\mathbb{Z}^2; \mathbb{C}^2),$$

where

$$L_{(p_1, p_2)}^2(\mathbb{C}/2\pi\mathbb{Z}^2, \mathbb{C}^2) := \{u \in L^2(\mathbb{C}/2\pi\mathbb{Z}^2) : \mathcal{L}_{(a_1, a_2)} u = e^{2\pi i(a_1 p_1 + a_2 p_2)} u, a_j \in \frac{1}{3}\mathbb{Z}\},$$

and  $\mathcal{L}_{(a_1, a_2)}$  is defined analogously to (6.3).

Using [BHZ22, Proposition 2.1] we see that the spectrum of  $T_k$  on  $L^2_{(0,0)}$  is the same, with multiplicities, as the spectrum of  $T_k$  on  $L^2_{(1,1)}$ , for  $k \in D(0, r) \setminus \{0\}$ , for  $r$  sufficiently small (so that we do not encounter other lattice points excluded in [BHZ22, (2.24)]).

We now define

$$A_k := \frac{1}{3} \mathcal{D}_k^{-1} \mathcal{V}_+ \mathcal{D}_k^{-1} \mathcal{V}_- : L^2_{(1,1)}(\mathbb{C}/2\pi\mathbb{Z}^2; \mathbb{C}) \rightarrow L^2_{(1,1)}(\mathbb{C}/2\pi\mathbb{Z}^2; \mathbb{C}),$$

$$L^2_{(p_1, p_2)}(\mathbb{C}/2\pi\mathbb{Z}^2; \mathbb{C}) := \{u \in L^2 : u(z + 2\pi(a_1, a_2)) = e^{2\pi i(a_1 p_1 + a_2 p_2)} u(z), \quad a_j \in \frac{1}{3}\mathbb{Z}\}.$$

(The strange looking factor of  $\frac{1}{3}$  makes the computation of traces easier – see [Be\*22, §3.3] and the next section here.)

The discussion above shows that

$$\begin{aligned} \text{Spec}_{L^2_{(0,0)}(\mathbb{C}/2\pi\mathbb{Z}^2, \mathbb{C}^2)}(T_k^2) \setminus \{0\} &= \text{Spec}_{L^2_{(1,1)}(\mathbb{C}/2\pi\mathbb{Z}^2, \mathbb{C}^2)}(T_k^2) \setminus \{0\} \\ &= 3 \text{Spec}_{L^2_{(1,1)}(\mathbb{C}/2\pi\mathbb{Z}^2, \mathbb{C})}(A_k) \setminus \{0\}, \end{aligned} \quad (7.2)$$

where  $k \in D(0, r) \setminus \{0\}$ , and the last inequality is meant in the sense of sets: multiplicities on the left are twice of the multiplicities on the right.

On the Fourier transform side we introduce

$$\begin{aligned} \mathcal{D}_k &:= \omega^2(D + k_1) - \omega(D + k_2), \quad \text{with } D = \text{diag}(\ell)_{\ell \in \mathbb{Z}} \\ \mathcal{V}_{\pm}(y) &:= J^{\pm} \otimes J^{\pm} + \omega J^{\mp 2} \otimes J^{\pm} + \omega^2 J^{\pm} \otimes J^{\mp 2}, \end{aligned} \quad (7.3)$$

where  $J$  is the right-shift  $J((a_n)_n) = (a_{n+1})_n$  – see [Be\*22, (3.17)]. The spaces  $L^2_{(p_1, p_2)}(\mathbb{C}/2\pi\mathbb{Z}^2; \mathbb{C})$  correspond to

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

The operator  $A_k$  is now (where we use the same notation)

$$A_k := \mathcal{D}_k^{-1} \mathcal{V}_+ \mathcal{D}_k^{-1} \mathcal{V}_- : \ell^2_{(1,1)} \rightarrow \ell^2_{(1,1)}. \quad (7.4)$$

We note that the mapping property is consistent with

$$\ell^2_{(1,1)} \xrightarrow{\mathcal{V}_-} \ell^2_{(2,2)} \xrightarrow{\mathcal{D}_k^{-1}} \ell^2_{(2,2)} \xrightarrow{\mathcal{V}_+} \ell^2_{(1,1)} \xrightarrow{\mathcal{D}_k^{-1}} \ell^2_{(1,1)}.$$

We also note that  $A_k$  is defined for  $k \in D(0, r)$  since  $D_0^{-1}$  is defined on  $\ell^2_{(p,p)}$ ,  $p \not\equiv 0 \pmod{3}$ . Since  $\mathbb{C} \ni k \rightarrow \mathcal{A}_k|_{\ell^2_{(1,1)}}$  is an analytic family of operators with compact resolvent and the spectrum is independent of  $k \in \mathbb{C} \setminus 3\Gamma^*$ , it follows that  $\text{Spec}(A_k) = \text{Spec}(A_0)$  [Ka80, Theorem 1.10]. From (7.2) we obtain, as sets,

$$\text{Spec}_{L^2_{(0,0)}}(T_p^2) \setminus \{0\} = 3 \text{Spec}_{\ell^2_{(1,1)}}(A_k) \setminus \{0\}, \quad p \in D(0, r) \setminus \{0\}, \quad k \in D(0, r), \quad (7.5)$$

with multiplicities on the left, twice the multiplicities on the right. Since  $k = 0$  is included in the set of possible  $k$  for  $A_k$ , we conclude together with [BHZ22, Theorem 6] that

$$\dim \ker_{\mathcal{H}}(D(\alpha)) = \dim \ker_{L^2_{(1,1)}}(A_0 - (3\alpha^2)^{-1}). \quad (7.6)$$

We also define operator  $\mathcal{A}_k$  using (7.4) but acting on all of  $\ell^2(\mathbb{Z}^2)$ . Then,

$$A_k := \mathcal{A}_k|_{\ell^2_{(1,1)}}, \quad (7.7)$$

We note that, unlike  $A_k$ , the operator  $\mathcal{A}_k$  is *not* well-defined for  $k = 0$ .

## 8. TRACES

The objective of this section is to prove Theorem 5 and to provide an algorithm for computing traces of powers of  $T_k$ .

For powers  $\ell = 2$  and  $\ell = 4$  in (6.8), the proof of [Be\*22, Theorem 3] relied heavily on explicit symmetries which led to a cancellation of most of the sums. The remaining ones could then be calculated by means of the cotangent series.

We were not able to find such symmetries for higher values of  $\ell$ . Hence, we use another method to obtain an explicit formula for traces of powers of  $T_k$ . Interestingly, the fact that the spectrum of  $T_k$  is independent of  $k$  plays a crucial role in the argument – see the application of Lemma 8.2 below.

We start by recalling the operator  $A_k := \mathcal{D}_k^{-1}\mathcal{V}_+\mathcal{D}_k^{-1}\mathcal{V}_- : \ell^2_{(1,1)} \rightarrow \ell^2_{(1,1)}$  introduced in (7.4), for which (7.5) and the symmetry  $\mathcal{A} = -\mathcal{A}$  (see [Be\*22] or [BHZ22, §2.5]) give

$$\mathrm{tr}(T_k^\ell) = \begin{cases} 2 \cdot 3^\ell \mathrm{tr}(A_k^{\ell/2}) & \text{for all } \ell \in 2\mathbb{N}, \quad \ell \geq 4, \\ 0 & \text{otherwise.} \end{cases}$$

As in [Be\*22, §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

$$J^{p,q} \Lambda J^{p',q'} = \Lambda_{p,q} J^{p+p',q+q'} = J^{p+p',q+q'} \Lambda_{-p',-q'}. \quad (8.1)$$

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

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

we see that

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

Using the relation (8.1), the diagonal part of  $\mathcal{A}_k^\ell$  is of the form

$$\begin{aligned} ((\mathcal{A}_k^\ell)_{ii})_{i \in \mathbb{Z}} &= \sum_{\pi \in \Theta_\ell} \omega^{m_\pi} \prod_{i=1}^{\ell} \Lambda_{\tilde{\alpha}_i, \tilde{\beta}_i} \Lambda_{\tilde{\gamma}_i, \tilde{\delta}_i}, \\ \pi &:= [(\alpha_1, \beta_1), (\gamma_1, \delta_1), (\alpha_2, \beta_2), \dots, (\gamma_\ell, \delta_\ell)], \end{aligned} \quad (8.2)$$

where

$$\begin{aligned}\tilde{\alpha}_i &= \sum_{j=1}^{i-1} \alpha_j + \gamma_j & \tilde{\beta}_i &= \sum_{j=1}^{i-1} \beta_j + \delta_j, & \tilde{\gamma}_i &= \alpha_i + \sum_{j=1}^{i-1} \alpha_j + \gamma_j, \\ \tilde{\delta}_i &= \beta_i + \sum_{j=1}^{i-1} \beta_j + \delta_j, & m_\pi &:= \frac{2}{3} \sum_{i=1}^{\ell} (\gamma_i + \beta_i).\end{aligned}\tag{8.3}$$

In (8.2), the sum is over elements of the finite set

$$\Theta_\ell := \left\{ \pi = [(\alpha_1, \beta_1), (\gamma_1, \delta_1), (\alpha_2, \beta_2), \dots, (\gamma_\ell, \delta_\ell)], \sum_{j=1}^{\ell} \alpha_j + \gamma_j = \sum_{j=1}^{\ell} \beta_j + \delta_j = 0, \right. \\ \left. (\alpha_i, \beta_i) \in \{(1, 1), (-2, 1), (1, -2)\}, (\gamma_i, \delta_i) \in \{(-1, -1), (2, -1), (-1, 2)\} \right\}.\tag{8.4}$$

Using (8.2), the diagonal part of  $A_k^\ell$ , defined in (7.7), is of the form

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

where  $\Lambda'$  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

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

Since most of the series we consider are *not* absolutely convergent, it is essential to specify orders of summation. For that we put

$$\mathcal{L} := \mathbb{Z}\omega^2 + \mathbb{Z}\omega = \mathbb{Z} + \omega\mathbb{Z},\tag{8.5}$$

and define the following *principal value* summation:

$$\begin{aligned}\sum_{\gamma \in \mathcal{L}} f(\gamma) &:= \sum_{n \in \mathbb{Z}} \sum_{m \in \mathbb{Z}} f(n\omega^2 - m\omega) \\ &:= \lim_{N_2 \rightarrow +\infty} \left( \sum_{n=-N_2}^{N_2} \lim_{N_1 \rightarrow +\infty} \sum_{m=-N_1}^{N_1} f(m\omega^2 - n\omega) \right).\end{aligned}\tag{8.6}$$

For  $l \geq 2$ , we aim to compute the sum of diagonal elements of  $A_k^\ell$ ,

$$\mathrm{tr}(A_k^\ell) = \sum_{\pi \in \Theta_\ell} \sum_{\gamma \in \mathcal{L}} \omega^{m_\pi} \prod_{i=1}^{\ell} \frac{1}{\underbrace{(3\gamma + k + \gamma_{(\tilde{\alpha}_i, \tilde{\beta}_i)} + \mu)(3\gamma + k + \gamma_{(\tilde{\gamma}_i, \tilde{\delta}_i)} + \mu)}_{=: f_\pi(k+3\gamma)}},$$

where we introduced

$$\gamma_{(a,b)} := \omega^2 a - \omega b \text{ and } \mu := \omega^2 - \omega = -i\sqrt{3}$$

We start with a partial fraction decomposition of  $f_\pi$  and observe that the poles of  $f_\pi$  are given by

$$\begin{aligned} \gamma_{(\tilde{\alpha}_i, \tilde{\beta}_i)} + \mu, \quad (\tilde{\alpha}_i, \tilde{\beta}_i) &\equiv (0, 0) \pmod{3} \\ \gamma_{(\tilde{\gamma}_i, \tilde{\delta}_i)} + \mu, \quad (\tilde{\gamma}_i, \tilde{\delta}_i) &\equiv (1, 1) \pmod{3}. \end{aligned}$$

By summing over equivalent poles, we obtain

$$f_\pi(k) = \omega^{m_\pi} \left( \sum_{i=1}^{N_{\pi,1}} \left( \sum_{j=1}^{n_{i,\pi,1}} \frac{a_{i,j,\pi}}{(k + 3\gamma_{i,j,\pi}^{(1)} + \mu)^j} + \sum_{j=1}^{n_{i,\pi,2}} \frac{b_{i,j,\pi}}{(k + 3\gamma_{i,j,\pi}^{(2)} + 2\mu)^j} \right) \right), \quad (8.7)$$

where we separated the poles of  $f_\pi$  according to their congruence modulo 3.

We analyse  $f_\pi(k)$  by fixing  $j$  and summing over  $i$ ,  $\gamma$  and  $\pi$ . For that we define

$$\tau_{k,(\ell,j)} := \sum_{\pi \in \Theta_\ell} \left( \sum_{i=1}^{N_{\pi,1}} \sum_{\gamma \in \mathcal{L}} \frac{a_{i,j,\pi}}{(k + 3(\gamma_{i,j,\pi}^{(1)} + \gamma) + \mu)^j} + \sum_{i=1}^{N_{\pi,2}} \sum_{\gamma \in \mathcal{L}} \frac{b_{i,j,\pi}}{(k + 3(\gamma_{i,j,\pi}^{(2)} + \gamma) + 2\mu)^j} \right).$$

At first, this definition is formal since we do not know that the principal values of the series, in the sense of (8.6), exist. Hence, we need to investigate the convergence of the  $\tau_{k,(\ell,j)}$ . Once that is done, we will have

$$\text{tr}(A_k^\ell) = \sum_{j=1}^{2\ell} \tau_{k,(\ell,j)}. \quad (8.8)$$

We will then show (Lemma 8.1 below) that the only contribution to the sum comes from  $j = 1$ .

**8.1. Analysis of  $\tau_{k,(\ell,j)}$ .** If  $j \geq 3$ , then the sum is absolutely convergent. We can then use the fact that  $\gamma_i \in \mathcal{L}$  and a change of variables in the sums over  $\mathcal{L}$  to deduce that

$$\sum_{\pi \in \Theta_\ell} \sum_{i=1}^{N_{\pi,1}} \sum_{\gamma \in \mathcal{L}} \frac{a_{i,j,\pi}}{(k + 3(\gamma_{i,j,\pi}^{(1)} + \gamma) + \mu)^j} = \underbrace{\left( \sum_{\pi \in \Theta_\ell} \sum_{i=1}^{N_{\pi,1}} a_{i,j,\pi} \right)}_{=: a_j} \sum_{\gamma \in \mathcal{L}} \frac{1}{(3\gamma + k + \mu)^j},$$

we then introduce

$$\tilde{k} = k + \mu, \quad p_j(\tilde{k}) := \sum_{\gamma \in \mathcal{L}} \frac{1}{(3\gamma + \tilde{k})^j}, \quad \tilde{k} \notin 3\mathcal{L}. \quad (8.9)$$

We can rewrite the previous equation as

$$\sum_{\pi \in \Theta_\ell} \sum_{i=1}^{N_{\pi,1}} \sum_{\gamma \in \mathcal{L}} \frac{a_{i,j,\pi}}{(k + 3(\gamma_{i,j,\pi}^{(1)} + \gamma) + \mu)^j} = a_j p_j(\tilde{k}).$$

Similarly, we can write

$$\sum_{\pi \in \Theta_\ell} \sum_{i=1}^{N_{\pi,2}} \sum_{\gamma \in \mathcal{L}} \frac{b_{i,j,\pi}}{(k + 3(\gamma_{i,j,\pi}^{(2)} + \gamma) + \mu)^j} = b_j p_j(\tilde{k} + \mu),$$

where we denoted

$$b_j := \sum_{\pi \in \Theta_\ell} \sum_{i=1}^{N_{\pi,2}} b_{i,j,\pi}.$$

Thus, we have

$$\tau_{k,(\ell,j)} = a_j p_j(\tilde{k}) + b_j p_j(\tilde{k} + \mu).$$

Now, consider  $j = 2$ . Our goal is to obtain a similar decomposition for  $\tau_{k,(2,j)}$ . The sum is now no longer absolutely convergent but it is semi convergent, in the following sense: with the order of summation as in (8.6), we have

$$\sum_{\gamma \in \mathcal{L} \setminus \{0\}} \frac{1}{(3\gamma + \mu)^2} =: K,$$

this is for instance an easy consequence of the following expansion of the cosecant function:

$$\csc^2(z) = \sum_{k=-\infty}^{+\infty} \frac{1}{(z + \pi k)^2}, \quad z \notin \pi\mathbb{Z}.$$

With this notation we have

$$\sum_{\gamma \in \mathcal{L}} \frac{1}{(k + 3\gamma + 3\gamma_{i,j\pi}^{(2)} + \mu)^2} = \frac{1}{k^2} + \sum_{\gamma \in \mathcal{L} \setminus \{-\gamma_{i,j\pi}^{(2)}\}} \frac{1}{(3\gamma + 3\gamma_{i,j\pi}^{(2)} + k + \mu)^2} - \frac{1}{(3\gamma + 3\gamma_{i,j\pi}^{(2)} + \mu)^2} + K.$$

where we recognize the Weierstrass  $\wp$ -function of the lattice  $3\mathcal{L}$

$$\sum_{\gamma \in \mathcal{L}} \frac{1}{(k + 3\gamma + 3\gamma_{i,j\pi}^{(2)} + \mu)^2} = \wp(\tilde{k}) + K =: p_2(\tilde{k}). \quad (8.10)$$

Hence, we have shown that

$$\tau_{k,(\ell,2)} = \underbrace{\left( \sum_{\pi \in \Theta_\ell} \sum_{i=1}^{N_{\pi,1}} a_{i,2,\pi} \right)}_{=: a_2} p_2(\tilde{k}) + \underbrace{\left( \sum_{\pi \in \Theta_\ell} \sum_{i=1}^{N_{\pi,2}} b_{i,2,\pi} \right)}_{=: b_2} p_2(\tilde{k} + \mu).$$

This also implies that  $\tau_{k,(\ell,1)}$  is also well defined and that (8.8) holds.

**8.2. Main contribution to the trace.** We now show that in (8.8) only  $j = 1$  appear. The argument relies on the fact that the spectrum (and hence the traces) are independent of  $k$ .

**Lemma 8.1.** *Let  $\ell \geq 2$  then*

$$\mathrm{tr}(A_k^\ell) = \tau_{k,(\ell,1)}.$$

*Proof.* The results of §8.1 showed that

$$\mathrm{tr}(A_k^\ell) = \sum_{j=1}^{2\ell} \tau_{k,(\ell,j)} = \sum_{j \geq 2} a_j p_j(\tilde{k}) + \sum_{j \geq 2} b_j p_j(\tilde{k} + \mu) + \tau_{k,(\ell,1)},$$

and this value does not depend on  $k \notin \mathcal{L}$ . Equivalently, the trace does not depend on  $\tilde{k} := k + \mu$ ,  $\mu = \omega^2 - \omega = -i\sqrt{3}$ . We prove that it implies  $\mathrm{tr}(A_k^\ell) = \tau_{k,(\ell,1)}$  so that the computation of the full trace reduces to the computation of the sum of terms with  $j = 1$ .

For that we use the following standard result of complex analysis:

**Lemma 8.2.** *Let  $l(z)$  be an even elliptic function on  $\mathbb{C}/3\mathcal{L}$  with a single pole of multiplicity  $2j$  at 0. Then there exist a polynomial  $P$  of degree  $j$  such that*

$$P(\wp(z)) = l(z),$$

where  $\wp(z)$  is the Weierstrass function for the lattice  $3\mathcal{L}$ .

*Proof.* Let  $a_1, -a_1, a_2, -a_2, \dots, a_j, -a_j$  be the zeros of  $l$  counted with multiplicity and define  $Q(z) := \prod_{i=1}^j (z - l(a_i))$ . Then  $Q$  is a polynomial of degree  $j$  such that  $Q(\wp(z))$  is an elliptic function that have the same zeros and poles as  $l$  with same multiplicity. Taking  $P = \lambda Q$  with suitable choice of  $\lambda$  then gives  $l(z) = P(\wp(z))$ ,  $z \notin \mathcal{L}$ .  $\square$

We recall that the trace is a constant function of  $\tilde{k} \notin 3\mathcal{L}$  and thus it is in particular even as a function of  $\tilde{k}$ . Definitions (8.9) and (8.10) show that  $p_j(-\tilde{k}) = (-1)^j p_j(\tilde{k})$  and hence,

$$\mathrm{tr}(A_k^\ell) = \sum_{j=1}^{\ell} a_{2j} p_{2j}(\tilde{k}) + \frac{\sum_{j \geq 2} b_j p_j(\tilde{k} + \mu) + \sum_{j \geq 2} b_j p_j(-\tilde{k} + \mu)}{2} + \tau_{k,(\ell,1)}. \quad (8.11)$$

Lemma 8.1 and definitions (8.9), (8.10) then show that there exists a family of polynomials  $(P_j)_{1 \leq j \leq \ell} \in \mathbb{C}[X]$  of degree  $j$  such that

$$\forall 1 \leq j \leq \ell, \quad p_{2j}(z) = P_j(\wp(z)), \quad z \notin 3\mathcal{L}.$$

Such a family is linearly independent and we have

$$\sum_{j=1}^{\ell} \tau_{k,(\ell,2j)} = \sum_{j=1}^{\ell} a_{2j} P_j(\wp(\tilde{k})) + \frac{\sum_{j \geq 2} b_j p_j(\tilde{k} + \mu) + \sum_{j \geq 2} b_j p_j(-\tilde{k} + \mu)}{2}. \quad (8.12)$$

The term

$$\frac{1}{2} \left( \sum_{j \geq 2} b_j p_j(\tilde{k} + \mu) + \sum_{j \geq 2} b_j p_j(-\tilde{k} + \mu) \right) + \tau_{k,(\ell,1)}$$

is bounded when  $\tilde{k} \rightarrow 0$  and the sum of the two terms does not depend on  $\tilde{k} \notin 3\mathcal{L}$ . Combined with (8.12), this implies that  $Q(X) := \sum_{j=1}^{\ell} a_{2j} P_j(X)$  is a constant polynomial and we have  $a_{2j} = 0$ . We can use a similar argument to show that the  $b_{2j}$  are also zero. More precisely, we have proved that the full trace is in fact equal to

$$\text{tr}(A_k^{\ell}) = \sum_{j \geq 2} b_j p_j(\tilde{k} + \mu) + \tau_{k,(\ell,1)},$$

using variable  $\hat{k} := \tilde{k} + \mu = k + 2\mu$ , we get that the function  $\hat{k} \mapsto \sum_{j \geq 2} b_j p_j(\hat{k})$  is constant in a neighborhood of 0. It is in particular even so that  $b_{2j+1} = 0$  for all  $j$ 's. Thus, we get that the polynomial  $R(X) := \sum_{j=1}^{\ell} b_{2j} P_j(X)$  is constant which implies that all  $b_{2j}$ 's vanish by the linear independence of the  $P_j$ 's.

Hence, we have shown that  $\text{tr}(A_k^{\ell}) = \tau_{k,(\ell,1)}$ , completing the proof of Lemma 8.1.  $\square$

**8.3. Evaluation of the trace.** Lemma 8.1 shows that to evaluate our traces we have to study the sum

$$\tau_{k,(\ell,1)} := \sum_{\pi \in \Theta_{\ell}} \left( \sum_{i=1}^{N_{\pi,1}} \sum_{\gamma \in \mathcal{L}} \frac{\text{Res}(f_{\pi}, -3\gamma_{i,j,\pi}^{(1)} - \mu)}{k + 3(\gamma_{i,j,\pi}^{(1)} + \gamma) + \mu} + \sum_{i=1}^{N_{\pi,2}} \sum_{\gamma \in \mathcal{L}} \frac{\text{Res}(f_{\pi}, -3\gamma_{i,j,\pi}^{(2)} - 2\mu)}{k + 3(\gamma_{i,j,\pi}^{(2)} + \gamma) + 2\mu} \right)$$

and prove that it is semi-convergent and that the sum does not depend on  $\tilde{k} \notin 3\mathcal{L}$ . We shall start by regrouping the elements in  $\Theta_{\ell}$ . We therefore define

$$\sigma : \mathbb{Z} \times \mathbb{Z} \rightarrow \mathbb{Z}, \quad \sigma(m, n) = (-(n + m), m)$$

and satisfies

$$\gamma_{\sigma(m,n)} = \omega \gamma_{(m,n)}.$$

This implies that  $\sigma^3 = \text{id}$  and that the orbits under  $\sigma$  are of cardinality 3. We define

$$S_{\pi}(k) = \sum_{i=1}^{N_{\pi,1}} \sum_{\gamma \in \mathcal{L}} \frac{\text{Res}(f_{\pi}, -3\gamma_{i,j,\pi}^{(1)} - \mu)}{(k + 3(\gamma_{i,j,\pi}^{(1)} + \gamma) + \mu)^j} + \sum_{i=1}^{N_{\pi,2}} \sum_{\gamma \in \mathcal{L}} \frac{\text{Res}(f_{\pi}, -3\gamma_{i,j,\pi}^{(2)} - 2\mu)}{(k + 3(\gamma_{i,j,\pi}^{(2)} + \gamma) + 2\mu)^j}.$$

The convergence of  $S_{[\pi]}(k) = S_{\pi}(k) + S_{\sigma(\pi)}(k) + S_{\sigma^2(\pi)}(k)$ , follows from the following Lemma:

**Lemma 8.3.** *Let  $(\alpha, v) \in \mathbb{C} \times \mathbb{C}^*$  such that*

$$\forall n \in \mathbb{Z}, \quad (n - i\alpha)^2 \neq v^2.$$

*We then have*

$$\sum_{n=-\infty}^{+\infty} \frac{1}{(n - i\alpha)^2 - v^2} = \frac{-i [\pi \coth(\pi(\alpha + iv)) + \pi \coth(\pi(iv - \alpha))]}{2v}.$$

*Proof.* This follows from  $\pi \coth(\pi z) = z^{-1} + 2z \sum_{n=1}^{+\infty} (z^2 + n^2)^{-2}$ .  $\square$

From this lemma, we deduce the following result

**Lemma 8.4.** *For  $\gamma_1, \gamma_2 \in \mathcal{L}, k \notin 3\mathcal{L} - \mu$  such that  $\gamma_1 - \gamma_2 = 3\alpha\omega^2 - 3\beta\omega \in 3\mathcal{L}$ , we have, in the sense of (8.6),*

$$\sum_{\gamma \in \mathcal{L}} \frac{1}{3\gamma + \mu + \gamma_1 + k} - \frac{1}{3\gamma + \mu + \gamma_2 + k} = -\frac{2i\omega\pi\beta}{3}, \quad (8.13)$$

where  $\mu = \omega^2 - \omega$ .

*Proof.* Taking common denominators gives

$$\begin{aligned} S(m, k, \gamma_1, \gamma_2) &:= \sum_{n=-\infty}^{+\infty} \frac{1}{3n\omega^2 - 3m\omega + \mu + \gamma_1 + k} - \frac{1}{3n\omega^2 - 3m\omega + \mu + \gamma_2 + k} \\ &= \sum_{n=-\infty}^{+\infty} \frac{1}{9\omega} \frac{\gamma_2 - \gamma_1}{\left(n - m\omega^2 + \frac{\mu}{3} + \frac{\gamma_1 + \gamma_2}{6}\omega + \frac{k}{3}\omega\right)^2 - \left(\omega \frac{\gamma_1 - \gamma_2}{6}\right)^2}. \end{aligned}$$

Lemma 8.3 shows that the sum converges and

$$\begin{aligned} S(m, k, \gamma_1, \gamma_2) &= \frac{i\pi\omega}{3} \left[ \coth \left( i\pi \left( -m\omega^2 + \omega \frac{\gamma_1 - \gamma_2}{6} \right) + \beta_0 \right) \right. \\ &\quad \left. + \coth \left( i\pi \left( m\omega^2 + \omega \frac{\gamma_1 - \gamma_2}{6} \right) - \beta_0 \right) \right], \end{aligned}$$

where we put

$$\beta_0 := \frac{i\pi\omega}{3} \left( \frac{\gamma_1 + \gamma_2}{2} + k \right).$$

The coth function is  $i\pi$  periodic so if we write

$$\frac{\gamma_1 - \gamma_2}{6} = \frac{\alpha\omega^2 - \beta\omega}{2}, \alpha, \beta \in \mathbb{Z},$$

noting that  $\alpha \in \mathbb{Z}$ , we have

$$\begin{aligned} \coth \left( x + i\pi\omega \frac{\gamma_1 - \gamma_2}{6} \right) + \coth \left( -x + i\pi\omega \frac{\gamma_1 - \gamma_2}{6} \right) &= \coth \left( x + i\pi \frac{\alpha}{2} - i\pi\omega^2 \frac{\beta}{2} \right) \\ &\quad - \coth \left( x + i\pi \frac{\alpha}{2} + i\pi\omega^2 \frac{\beta}{2} \right). \end{aligned}$$

We want to find the  $N \rightarrow \infty$  limit of

$$\begin{aligned} \sum_{m=-N}^N S(m, k, \gamma_1, \gamma_2) &= \frac{i\pi\omega}{3} \sum_{m=-N}^N \left( \coth \left( i\pi\omega^2 m + \beta_1 - i\pi\omega^2 \frac{\beta}{2} \right) \right. \\ &\quad \left. - \coth \left( i\pi\omega^2 m + \beta_1 + i\pi\omega^2 \frac{\beta}{2} \right) \right), \end{aligned}$$

where we have put

$$\beta_1 := -\beta_0 + i\pi \frac{\alpha}{2}.$$

Now, because  $\beta \in \mathbb{Z}$ , we have a telescopic sum and

$$\begin{aligned} \sum_{m=-N}^N S(m, k, \gamma_1, \gamma_2) &= \frac{i\pi\omega}{3} \left[ \sum_{m=N+1}^{N+\beta} \coth \left[ i\pi\omega^2 \left( \frac{\beta}{2} + m \right) + \beta_1 \right] \right. \\ &\quad \left. - \sum_{m=-N}^{-N+\beta-1} \coth \left[ i\pi\omega^2 \left( m + \frac{\beta}{2} \right) + \beta_1 \right] \right]. \end{aligned}$$

Since  $\operatorname{Re} i\pi\omega^2 = \sqrt{3} > 0$ , the terms in the first and second sum tend to 1 and  $-1$  as  $N \rightarrow +\infty$ , respectively. This completes the proof of (8.13).  $\square$

To compute the trace, we need to show that  $\tau_{k,(\ell,1)}$  decomposes into sums appearing in the previous lemma. This follows from the following two observations on the residues of  $f_\pi$ :

- (i) For all  $i$  between  $1 \leq i \leq N_\pi$ , we have  $\operatorname{Res}(f_\pi, -\gamma(i)) \in \mathbb{Q}(\omega)$ .  
Indeed, we just need to consider the partial expansion of  $f_\pi \in [\mathbb{Q}(\omega)](X)$  (rational functions of  $X$  with coefficients in the field  $\mathbb{Q}(\omega)$ ) and then use the uniqueness of that expansion.

Therefore, we can assume that  $\forall 1 \leq i \leq N_\pi$ , we have

$$\operatorname{Res}(f_\pi, -\gamma_i) = a_i + \omega b_i, \quad a_i, b_i \in \mathbb{Z}. \quad (8.14)$$

(We can always multiply  $f_\pi$  by an integer big enough).

- (ii) We recall that  $\sigma(n, m) \equiv (n, m) \pmod{3}$  if  $(m, n) \equiv (1, 1) \pmod{3}$  or  $(m, n) \equiv (0, 0) \pmod{3}$ .

For a  $\pi = [(\alpha_1, \beta_1), (\gamma_1, \delta_1), (\alpha_2, \beta_2), \dots, (\gamma_\ell, \delta_\ell)] \in \Theta_\pi$ , we define

$$\sigma(\pi) = [\sigma(\alpha_1, \beta_1), \sigma(\gamma_1, \delta_1), \sigma(\alpha_2, \beta_2), \dots, \sigma(\gamma_\ell, \delta_\ell)].$$

Note that  $\sigma(\pi) \in \Theta_\ell$ . Moreover, we have  $m_{\sigma(\pi)} \equiv m_\pi - l \pmod{3}$ . Because of the relation  $\gamma_{\sigma(m,n)} = \omega \gamma_{(m,n)}$ , we see that

$$\operatorname{Res}(f_{\sigma(\pi)}, \gamma_{\sigma(m,n)}) = \omega^{-l} \omega^{l+1} \operatorname{Res}(f_\pi, \gamma_{(m,n)}) = \omega \operatorname{Res}(f_\pi, \gamma_{(m,n)}).$$

We then conclude that

$$\sum_{i=0}^2 \operatorname{Res}(f_{\sigma^i(\pi)}, \gamma_{\sigma^i(m,n)}) = \sum_{i=0}^2 \omega^i \operatorname{Res}(f_\pi, \gamma_{(m,n)}) = 0.$$

Now, for each pole  $\gamma_0$ , we write

$$\frac{\operatorname{Res}(f_\pi, -\gamma_0)}{(3\gamma + \tilde{k} + \gamma_0)} = \underbrace{\frac{1}{(3\gamma + \tilde{k} + \gamma_0)} + \dots + \frac{1}{(3\gamma + \tilde{k} + \gamma_0)}}_{a_i \text{ - times}} + \underbrace{\frac{\omega}{(3\gamma + \tilde{k} + \gamma_0)} + \dots + \frac{\omega}{(3\gamma + \tilde{k} + \gamma_0)}}_{b_i \text{ - times}}.$$

Using (ii), if we consider the orbit  $(\gamma_0, \omega\gamma_0, \omega^2\gamma_0)$ , we can pair each  $+1$  with a  $-1$  and each  $\omega$  with a  $-\omega$  so that we have decomposed our  $S_{[\pi]}$  into sums that we can calculate with the help of Lemma 8.4.

We summarize our findings in the following theorem.

**Theorem 8.** *Let  $\ell \geq 2$  and  $\Theta_\ell$  be as in (8.4) with coefficients  $\tilde{\alpha}_i, \tilde{\delta}_i, m_\pi$  as in (8.3). Then the traces are given by*

$$\mathrm{tr}(A_k^\ell) = -\frac{2i\omega\pi}{9} \sum_{\pi \in \Theta_\ell} \sum_{(\eta_i, \varepsilon_i) \in \{(\tilde{\alpha}_i, \tilde{\beta}_i), (\tilde{\gamma}_i, \tilde{\delta}_i), 1 \leq i \leq \ell\}} \mathrm{Res}(f_\pi, -\gamma_{(\eta_i, \varepsilon_i)}) \varepsilon_i,$$

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

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

*Proof.* In (8.14) we can suppose, without loss of generality, that  $a_i, b_i \geq 0$ . As discussed before the Theorem, each time a  $1$  is paired with a  $-1$ , Lemma 8.4 gives a contribution of  $-2i\omega(\varepsilon_i + 1)/9$  coming from  $\gamma_i = \gamma_{(\eta_i, \varepsilon_i)} + \mu$ . When we sum up all these contributions, we get

$$\frac{-2i\pi\omega}{9}(\varepsilon_i + 1)(a_i + \omega b_i) = \frac{-2i\pi\omega}{9}(\varepsilon_i + 1)\mathrm{Res}(f_\pi, -\gamma_i)$$

and using the fact that the sum of residues of  $S_{[\pi]}$  is zero, since the function obeys a growth bound  $O(R^{-4})$  when  $R \rightarrow +\infty$ , this finally yields our formula.  $\square$

We are now able to finish

*Proof of Theorem 5.* For symmetry reasons the trace has to be real. We can therefore write

$$\mathrm{tr}(A_k^\ell) = \mathrm{Re} \left( -\frac{2i\omega\pi}{9} \sum_{\pi \in \Theta_\ell} \sum_{i=1}^{N_\pi} \mathrm{Res}(f_\pi, -\gamma_{(\eta_i, \varepsilon_i)}) \varepsilon_i \right).$$

Using the fact that  $\mathrm{Res}(f_\pi, -\gamma_{(\eta_i, \varepsilon_i)}) \in \mathbb{Q}(\omega)$ , we deduce that  $\mathrm{tr}(A_k^\ell) = \pi/\sqrt{3}q_\ell$ ,  $q_\ell \in \mathbb{Q}$ .  $\square$

**Remark.** We observe that the final formula does not depend on  $\mu = 1\omega^2 - 1\omega$  (which comes from  $(1, 1)$  in  $\ell^2_{(1,1)}$ ). Indeed, the same computation could be used to study the traces of restriction of  $\mathcal{A}_k$  on any subspace  $\ell^2_{(p,q)}$ . The result would be the same and we therefore arrive again at the fact that of these restriction has the same spectrum (see [BHZ22, Proposition 2.1] The spectrum of  $A_0$  is equal to the spectrum of  $\mathcal{A}_k$  but with 9-fold multiplicity.

9. INFINITELY MANY MAGIC ANGLES

We start by showing that the chiral Hamiltonian exhibits infinitely many magic angles.

*Proof of Theorem 6.* We start by observing that since  $\pi$  is transcendental, so is  $\pi/\sqrt{3}$ . 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

$$e_n(\lambda_1, \dots, \lambda_N) = (-1)^n \sum_{\substack{m_1 + 2m_2 + \dots + nm_n = n \\ m_1 \geq 0, \dots, m_n \geq 0}} \prod_{i=1}^n \frac{(-\operatorname{tr} A_k^{2i})^{m_i}}{m_i! i^{m_i}} \quad (9.1)$$

where  $e_n = 0$  for  $n > N$ . Theorem 5 shows that

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

The power  $m_1 \cdots m_n$  from sequences allowed in (9.1) is maximized by the unique choice  $m = (n, 0, \dots, 0)$ . The Newton identities for  $n > N$  then imply that the transcendental number  $\pi/\sqrt{3}$  is a root of a polynomial with rational coefficients. But then all these coefficients vanish, and in particular  $\operatorname{tr} A_k^2 = 0$ , which contradicts [Be\*22, Theorem 3].  $\square$

The previous proof can be generalized in the following way. For  $n \in 3\mathbb{Z} + 1$ , consider functions

$$f_n(z) := \sum_{k=0}^2 \omega^k \exp\left(\frac{n}{2} (z\bar{\omega}^k - \bar{z}\omega^k)\right).$$

Fix a  $N \geq 0$  and put

$$U(z) = \sum_{|n| \leq N, n \equiv 1 \pmod{3}} a_n f_n(z). \quad (9.2)$$

Then  $U(z)$  has symmetries (6.1) where the first two are always satisfied and the last one hold for  $a_n \in \mathbb{R}$ .

We also know (see [BHZ22, Theorem 4]) that the spectrum of  $T_k$  is independent of  $k$ . It is easy to see that the formula for the traces generalizes to this case (we only need to change  $\Theta_\ell$  set and account for the coefficients  $a_n$  in the formula). We deduce the following fact. 1' Let  $N \geq 0$ , and  $(a_n)_{|n| \leq N} \in (\mathbb{Q} + i\mathbb{Q})^{2N+1}$ , and define  $U$  by (9.2). Then for  $l \geq 2$  and for  $k \notin \mathcal{L}$ , we have

$$\operatorname{tr}(A_k^\ell) = q_\ell \frac{\pi}{\sqrt{3}} \quad q_\ell \in \mathbb{Q} + i\mathbb{Q}.$$

Since the existence of a magic  $\alpha$  is equivalent to the existence of  $l \geq 2$  such that  $\text{tr}(A_k^l) \neq 0$ , we deduce the following theorem.

**Theorem 9.** *Let  $N \geq 0$ ,  $a = (a_n)_{|n| \leq N} \in (\mathbb{Q} + i\mathbb{Q})^{2N+1}$ , and define  $U$  by (9.2). If  $\mathcal{A}_a$  in the set of magic angles for the potential  $U$ , then we have*

$$\mathcal{A}_a \neq \emptyset \implies |\mathcal{A}_a| = +\infty.$$

*In particular, the above implication holds on a generic (in the sense of Baire) set of coefficients  $a = (a_n)_{|n| \leq N} \in \mathbb{C}^{2N+1}$  that contains  $(\mathbb{Q} + i\mathbb{Q})^{2N+1}$ .*

*Proof.* Proof of Theorem 6 and Theorem 9 show that the conclusion holds for  $(a_n)_{|n| \leq N} \in (\mathbb{Q} + i\mathbb{Q})^{2N+1}$ . Thus, let  $a = (a_n)_{|n| \leq N} \in \mathbb{C}^{2N+1}$  and assume that  $\mathcal{A}_a \neq \emptyset$ . 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  $\mathcal{A}_b \neq \emptyset$ . Take  $q = (q_n)_{|n| \leq N} \in (\mathbb{Q} + i\mathbb{Q})^{2N+1} \cap \Omega_a$  for which we then have  $|\mathcal{A}_q| = \infty$ . Continuity of eigenvalues of  $T_k$  as the potential  $U$  changes shows that the  $V_{m,a} := \{b \in \Omega_a : |\mathcal{A}_b| \geq m\}$  is open and dense in  $\Omega_a$ . Hence, the set of 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  $(\mathbb{Q} + i\mathbb{Q})^{2N+1}$ .  $\square$

## 10. FREDHOLM DETERMINANTS AND THE FIRST MAGIC ANGLE

We start by defining the regularized Fredholm determinant

$$\det_2(1 - 3\alpha^2 A_k) = \prod_{\lambda \in \text{Spec}(A_k)} E_1(3\alpha^2 \lambda) \text{ with } E_1(z) = (1 - z)e^z \quad (10.1)$$

where the product respects multiplicities. By definition  $\det_2(1 - 3\alpha^2 A_k) = 0 \Leftrightarrow \alpha^{-1} \in \text{Spec}(T_k) \setminus \{0\}$ . The symmetry of the spectrum of  $A_k$ ,  $\text{Spec}(A_k) = \overline{\text{Spec}(A_k)}$ , implies that  $\alpha \mapsto \det(1 - \alpha^2 A_k)$  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 10.1.** *The determinant  $\mathbb{C} \ni \alpha \mapsto \det(1 - 3\alpha^2 A_k)$  in (10.1) is an entire function, independent of  $k \in \mathbb{C}$ , which for any  $n, m \in \mathbb{N}_0$  satisfies*

$$\left| \partial_\alpha^m \det(1 - 3\alpha^2 A_k) - \sum_{k=0}^n \partial_\alpha^m \mu_k \frac{(-3)^k \alpha^{2k}}{k!} \right| \leq \sum_{j=n+1}^{\infty} \partial_{|\alpha|}^m \left( \frac{\sqrt{e} \inf_{k \in \mathbb{C}} \|A_k\|_2 3 |\alpha|^2}{j} \right)^j$$

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

$$\mu_j = \det \begin{pmatrix} 0 & j-1 & 0 & \cdots & 0 \\ \sigma_2 & 0 & j-2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \sigma_{j-1} & \sigma_{j-2} & \cdots & 0 & 1 \\ \sigma_j & \sigma_{j-1} & \sigma_{j-2} & \cdots & 0 \end{pmatrix}, \text{ with } \sigma_j = \text{tr } A_k^j. \quad (10.2)$$

*Proof.* The expression (10.1) is well-defined since  $A_k$  is a Hilbert-Schmidt operator. Indeed, since  $|E_1| \leq e^{\frac{|z|^2}{2}}$  for  $z \in \mathbb{C}$  and  $\sum_{\lambda \in \text{Spec}(A_k)} |\lambda|^2 \leq \|A_k\|_2^2$ , we conclude that

$$|\det(1 - 3\alpha^2 A_k)| \leq \exp\left(\frac{9|\alpha|^4 \|A_k\|_2^2}{2}\right).$$

Cauchy estimates show

$$|\mu_k| \leq \frac{k!}{|\alpha|^{2k}} \exp\left(\frac{9|\alpha|^4 \|A_k\|_2^2}{2}\right)$$

which is optimized at  $3|\alpha|^2 = \frac{\sqrt{k}}{\|A_k\|_2}$ , such that

$$|\mu_k| \leq \frac{\|A_k\|_2^k e^{k/2} k!}{k^k}.$$

The Taylor coefficients  $\mu_k$  are then given by the Plemelj-Smithies formula [Si77] stated in (10.2). 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  $A_{\mathbf{0}} = (A_{\mathbf{0}}(n))_{n \in \mathbb{Z}^2}$  and let  $P_m$  be the projection onto  $(3\{-m, -m+1, \dots, m\} + 1)^2$ , then

$$\|A_{\mathbf{0}}\|_2 \leq \|P_M A_{\mathbf{0}}\|_2 + \|(\text{id} - P_M) A_{\mathbf{0}}\|_2.$$

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

$$\|P_M A_{\mathbf{0}}\|_2 = \sqrt{\text{tr}(P_M A_{\mathbf{0}} A_{\mathbf{0}}^* P_M)} \leq 5/3 \text{ for } M = 200.$$

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

$$\|(\text{id} - P_M) A_{\mathbf{0}}\|_2 \leq 9 \|(\text{id} - P_M) (\mathcal{D}_{\mathbf{0}}^{-1})_{\ell_{(1,1)}^2 \rightarrow \ell_{(1,1)}^2}\|_4 \|(\mathcal{D}_{\mathbf{0}}^{-1})_{\ell_{(2,2)}^2 \rightarrow \ell_{(2,2)}^2}\|_4. \quad (10.3)$$

We recall that by definition

$$\|(\mathcal{D}_{\mathbf{0}}^{-1})_{\ell_{(1,1)}^2 \rightarrow \ell_{(1,1)}^2}\|_4 = \left( \sum_{m \in (3\mathbb{Z}+1)^2} |\omega^2 m_1 - \omega m_2|^{-4} \right)^{1/4}.$$

A simple change of variables shows that  $\|(\mathcal{D}_{\mathbf{0}}^{-1})_{\ell_{(1,1)}^2 \rightarrow \ell_{(1,1)}^2}\|_4 = \|(\mathcal{D}_{\mathbf{0}}^{-1})_{\ell_{(2,2)}^2 \rightarrow \ell_{(2,2)}^2}\|_4$ . 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

$$\|(\mathcal{D}_{\mathbf{0}}^{-1})_{\ell_{(2,2)}^2 \rightarrow \ell_{(2,2)}^2}\|_4 = \frac{1}{\sqrt{3}} \left( \sum_{m \in \mathbb{Z}^2} \frac{1}{g(m)^2} \right)^{1/4}.$$

While an explicit computation shows using exact symbolic calculations

$$\sum_{|m|_\infty \leq 6} \frac{1}{g(m)^2} \leq \frac{24}{7} \quad (10.4)$$

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

$$\sum_{|m|_\infty \geq 7} \frac{1}{g(m)^2} \leq \int_6^\infty \frac{2\pi r}{(r^2+5^2)^2} dr = \frac{\pi}{61} \Rightarrow \|(\mathcal{D}_0^{-1})_{\ell_{(2,2)}^2 \rightarrow \ell_{(2,2)}^2}\|_4 \leq \left(\frac{8}{21} + \frac{\pi}{549}\right)^{1/4}. \quad (10.5)$$

Inserting this estimate into (10.3), we find along the lines of (10.5)

$$\begin{aligned} \|(\text{id} - P_M)A_0\|_2 &\leq \frac{71}{10} \|(\text{id} - P_M)(\mathcal{D}_0^{-1})_{\ell_{(1,1)}^2 \rightarrow \ell_{(1,1)}^2}\|_4 \\ &\leq \frac{71}{10} \frac{1}{\sqrt{3}} \left( \int_{200}^\infty \frac{2\pi r}{(r^2 + 199^2)^2} dr \right)^{1/4} < \frac{1}{3}, \end{aligned} \quad (10.6)$$

which shows that  $\|A_0\|_2 < 2$ .

□

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 7. Indeed, (7.6) implies together with [BHZ22, Theorem 6] the existence of a gap between the two flat bands of the Hamiltonian and the remaining bands.

**Proposition 10.2.** *There exists a simple real eigenvalue  $\frac{1}{3\alpha_*^2}$  to the operator  $A_k$ , independent of  $k \in \mathbb{C}$ , with  $\alpha_* \in (0.583, 0.589)$  such that  $(\frac{1}{3\alpha_*^2}, \infty) \subset \mathbb{R} \setminus \text{Spec}(A_k)$ .*

*Proof.* To see that this is the first real magic angle, we first notice that

$$\|A_0\| \leq 9 \|(\mathcal{D}_0^{-1})_{\ell_{(1,1)}^2 \rightarrow \ell_{(1,1)}^2}\|^2 = 3.$$

This estimate shows that  $\alpha \in \mathbb{R}^+$  with  $1/(3\alpha^2) \in \text{Spec}(A_0)$  satisfies  $\alpha \geq \frac{1}{3}$ . The traces recorded in Table 1 are then relevant to prove the existence of a magic angle.

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

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

Evaluating the bound for  $N = 7$  and  $\nu = \sqrt{e}\|A_0\|_2\alpha^2$  we obtain for  $\alpha = 0.6$  that  $r_0 \leq 2 \cdot 10^{-2}$  and  $r_1 \leq 0.5$ . The existence of a root follows from studying

$$f(\alpha) := \sum_{k=0}^6 \mu_k \frac{(-3)^k \alpha^{2k}}{k!}, \quad \sup_{\alpha \in (1/3, \beta)} f'(\alpha) \leq g(\beta = 0.6) := \sum_{k=2}^{20} a_k(\beta)$$

| $p$ | $\sigma_p \frac{\sqrt{3}}{\pi}$ | $p$ | $\sigma_p \frac{\sqrt{3}}{\pi}$ |
|-----|---------------------------------|-----|---------------------------------|
| 1   | 2/9                             | 5   | 9560/20007                      |
| 2   | 4/9                             | 6   | 245120/527877                   |
| 3   | 32/63                           | 7   | 1957475168/4337177481           |
| 4   | 40/81                           | 8   | 13316086960/30360242367         |

TABLE 1. Traces of  $A_k$   $\sigma_p = \text{tr}(A_k^p)$ , where  $\sigma_1$  is not absolutely summable as  $A_k$  is not of trace-class.

where

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

One then checks (using computations involving integers only)

$$f(0.583) > 2.5 \cdot 10^{-2}, \quad f(0.589) < -2.5 \cdot 10^{-2}, \quad \text{and } g(0.6) < -\frac{7}{10}.$$

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

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