Algebraic area distribution of two-dimensional random walks and the Hofstadter model

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UNIVERSITÉ PARIS SUD
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École doctorale n°564 Physique en Île-de-France
Spécialité de doctorat: Physique

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Shuang WU

Composition du Jury :

M. Sergei Matveenko Professeur, L.D. Landau Institute for Theoretical Physics	Rapporteur
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M. Olivier Giraud Chargé de Recherche, Université Paris-Sud (LPTMS)	Invité

Titre : titre (en français).....

Distribution de l'aire algébrique enclose par les marches aléatoires bi-dimensionnelles et le modèle de Hofstadter..... ....

Mots clés : l'aire algébrique, les marches aléatoires, le modèle de Hofstadter

Cette thèse porte sur le modèle de Hofstadter i.e., un électron qui se déplace sur un réseau carré couplé à un champ magnétique homogène et perpendiculaire au réseau. Son spectre en énergie est l'un des célèbres fractals de la physique quantique, connu sous le nom "le papillon de Hofstadter". Cette thèse consiste en deux parties principales: la première est l'étude du lien profond entre le modèle de Hofstadter et la distribution de l'aire algébrique entourée par les marches aléatoires sur un réseau carré bidimensionnel. La seconde partie se concentre sur les caractéristiques spécifiques du papillon de Hofstadter et l'étude de la largeur de bande du spectre. On a trouvé une formule exacte pour la trace de l'Hamiltonien de Hofstadter en termes des coefficients de Kreft, et également pour les moments supérieurs de la largeur de bande.

Cette thèse est organisée comme suit. Dans le chapitre 1, on commence par la motivation de notre travail. Une introduction générale du modèle de Hofstadter ainsi que des marches aléatoires sera présentée. Dans le chapitre 2, on va montrer comment utiliser le lien entre les marches aléatoires et le modèle de Hofstadter. Une méthode de calcul de la fonction génératrice de l'aire algébrique entourée par les marches aléatoires planaires sera expliquée en détail. Dans le chapitre 3, on va présenter une autre méthode pour étudier ces questions en utilisant le point de vue "point spectrum traces" et retrouver la trace de Hofstadter complète. De plus, l'avantage de cette construction est qu'elle peut être généralisée au cas de "l'amost Mathieu opérateur". Dans le chapitre 4, on va introduire la méthode développée par D.J.Thouless pour le calcul de la largeur de bande du spectre de Hofstadter. En suivant la même logique, on va montrer comment généraliser la formule de la largeur de bande de Thouless à son n-ième moment, à définir plus précisément ultérieurement.

Title : (titre en anglais).... Algebraic area distribution of two-dimensional random walks and the Hofstadter mode..... ....

Keywords : Hofstadter mode, random walks, Algebraic area

This thesis is about the Hofstadter model, i.e., a single electron moving on a two-dimensional lattice coupled to a perpendicular homogeneous magnetic field. Its spectrum is one of the famous fractals in quantum mechanics, known as the Hofstadter's butterfly. There are two main subjects in this thesis: the first is the study of the deep connection between the Hofstadter model and the distribution of the algebraic area enclosed by two-dimensional random walks. The second focuses on the distinctive features of the Hofstadter's butterfly and the study of the bandwidth of the spectrum. We found an exact expression for the trace of the Hofstadter Hamiltonian in terms of the Kreft coefficients, and for the higher moments of the bandwidth. This thesis is organized as follows. In chapter 1, we begin with the motivation of our work and a general introduction to the Hofstadter model as well as to random walks will be presented. In chapter 2, we will show how to use the connection between random walks and the Hofstadter model. A method to calculate the generating function of the algebraic area distribution enclosed by planar random walks will be explained in details. In chapter 3, we will present another method to study these issues, by using the point spectrum traces to recover the full Hofstadter trace. Moreover, the advantage of this construction is that it can be generalized to the almost Mathieu operator. In chapter 4, we will introduce the method which was initially developed by D.J.Thouless to calculate the bandwidth of the Hofstadter spectrum. By following the same logic, I will show how to generalize the Thouless bandwidth formula to its n-th moment, to be more precisely defined later.

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To my parents

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Je remercie également mes parents qui m'ont soutenu tout au long de mes études.

Résumé simplifié

Cette thèse porte sur le modèle de Hofstadter i.e., un électron qui se déplace sur un réseau carré couplé à un champ magnétique homogène et perpendiculaire au réseau. Son spectre en énergie est l'un des célèbres fractals de la physique quantique, connu sous le nom "le papillon de Hofstadter". Cette thèse consiste en deux parties principales: la première est l'étude du lien profond entre le modèle de Hofstadter et la distribution de l'aire algébrique entourée par les marches aléatoires sur un réseau carré bidimensionnel. La seconde partie se concentre sur les caractéristiques spécifiques du papillon de Hofstadter et l'étude de la largeur de bande du spectre. On a trouvé une formule exacte pour la trace de l'Hamiltonien de Hofstadter en termes des coefficients de Kreft, et également pour les moments supérieurs de la largeur de bande.

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Foreword

This thesis is about the Hofstadter model, i.e., a single electron moving on a two-dimensional lattice coupled to a perpendicular homogeneous magnetic field. Its spectrum is one of the famous fractals in quantum mechanics, known as the Hofstadter's butterfly. There are two main subjects in this thesis: the first is the study of the deep connection between the Hofstadter model and the distribution of the algebraic area enclosed by two-dimensional random walks. The second focuses on the distinctive features of the Hofstadter's butterfly and the study of the bandwidth of the spectrum. We found an exact expression for the trace of the Hofstadter Hamiltonian in terms of the Kreft coefficients, and for the higher moments of the bandwidth.

This thesis is organized as follows. In chapter 1, we begin with the motivation of our work and a general introduction to the Hofstadter model as well as to random walks will be presented. In chapter 2, we will show how to use the connection between random walks and the Hofstadter model. A method to calculate the generating function of the algebraic area distribution enclosed by planar random walks will be explained in details. In chapter 3, we will present another method to study these issues, by using the point spectrum traces to recover the full Hofstadter trace. Moreover, the advantage of this construction is that it can be generalized to the almost Mathieu operator. In chapter 4, we will introduce the method which was initially developed by D.J.Thouless to calculate the bandwidth of the Hofstadter spectrum. By following the same logic, I will show how to generalize the Thouless bandwidth formula to its n-th moment, to be more precisely defined later.

Publication List

The original results of this thesis are based on the three following publications :

- S. Ouvry, S. Wagner and S. Wu: **On the algebraic area of lattice walks and the Hofstadter model**. – *Journal of Physics A: Mathematical and Theoretical.* DOI: 10.1088/1751-8113/49/49/495205, arXiv:1606.03273
- S. Ouvry and S. Wu: **Thouless bandwidth formula in the Hofstadter model**. – *Journal of Physics A: Mathematical and Theoretical*, DOI: 10.1088/1751-8121/aa9042, arXiv:1703.09634
- S. Ouvry, S. Wagner and S. Wu: **Hofstadter point spectrum trace and the Almost Mathieu operator**. – *Journal of Mathematical Physics*, DOI: 10.1063/1.5020147, arXiv:1711.03900

Résumé en français

Vue d'ensemble et motivations

En 1976, un article sur les niveaux d'énergie d'un seul électron se déplaçant dans un réseau bidimensionnel couplé à un champ magnétique a été publié. Cet article trace l'une des premières fractales quantiques, connu sous le nom de papillon de Hofstadter (**??**), nommé d'après son découvreur, Douglas Hofstadter. Cependant, l'étude de ce modèle est apparue beaucoup plus tôt. Felix Bloch [1] est le pionnier avec l'une des premières contributions. En 1929, seulement cinq ans après que Erwin Schrödinger dérivé l'équation de Schrödinger, Bloch a publié un article sur la structure de bande d'un seul électron dans un réseau cristallin soumis à un potentiel périodique. $V(\mathbf{r}) = V(\mathbf{r}+\mathbf{T})$ (où la période $\mathbf{T} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}$ avec n_1, n_2, n_3 sont des entiers et $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ sont les vecteurs de base du réseau).Son Hamiltonien est $H = \frac{\mathbf{p}^2(\mathbf{r})}{2m} + V(\mathbf{r})$. Le théorème de Bloch déclare que la fonction d'onde d'un tel électron peut être écrite comme $\psi_{\boldsymbol{k},n}(\mathbf{r}) = u_{\boldsymbol{k},n}(\boldsymbol{r})e^{i\boldsymbol{kr}}$, où $\boldsymbol{k}$ est le vecteur d'onde et $u_{\boldsymbol{k},n}(\boldsymbol{r}+\boldsymbol{T}) = u_{\boldsymbol{k},n}(\boldsymbol{T})$ est une fonction périodique avec la même périodicité que le potentiel $V(\mathbf{r})$. En utilisant la fonction d'onde de Bloch et la transformation de Fourier, on peut résoudre la fonction propre $H\psi_{\boldsymbol{k},n} = E_n(\boldsymbol{k})\psi_{\boldsymbol{k},n}$ (n est l'indice de la bande). Il se trouve le spectre d'énergie de la fonction d'onde de Bloch n'est pas continue. En fait, la présence du réseau (le potentiel périodique) brise l'énergie (l'énergie cinétique de l'électron libre) en morceaux. Chaque pièce s'appelle une bande d'énergie et les espaces entre eux sont des régions d'énergie interdites (voir fig. 1.1, le cas le plus simple: mélange des deux premières bandes uniquement).

D'autre part, presque dans la même période, Landau [2] travaillait sur le modèle quantique d'un électron libre dans un champ magnétique perpendiculaire $\mathbf{B}$ avec l'Hamiltonien $H = \frac{(\mathbf{p}-e\mathbf{A}/\hbar)^2}{2m}$. On peut introduire $\boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}/\hbar$ avec la relation de commutation $[\pi_x, \pi_y] = ie\hbar B$, et définir les opérateurs $a = \frac{1}{2e\hbar B}(\pi_x - i\pi_y)$ et $a^+ = \frac{1}{2e\hbar B}(\pi_x + i\pi_y)$ avec $[a, a^+] = 1$. a et a^+ sont similaires aux opérateurs de création et d'annihilation d'un oscillateur harmonique. En utilisant les substitutions ci-dessus, l'Hamiltonien devient $H = \frac{\boldsymbol{\pi}^2}{2m} = \hbar\omega_B(a^+a + \frac{1}{2})$ avec $\omega_B = eB/m$ la fréquence cyclotron. Les énergies propres quantifiées sont maintenant connues sous le nom de niveaux de Landau: $E_n = \hbar\omega_B(n+1/2)$ où n est l'indice du niveaux de Landau. Ainsi, en présence d'un champ magnétique uniforme, les énergies sont régulièrement espacées et l'intervalle entre chaque niveau est proportionnel au champ magnétique.(voir fig. 1.2).

La question naturelle est de combiner ces deux problèmes: que se passera-t-il si quelqu'un pose un électron sur un réseau discret et lui applique ensuite un champ magnétique perpendiculaire? Beaucoup de physiciens se sont intéressés à ce problème depuis des décennies. Parmi eux, un modèle simple conçu par Onsager et Peierls [3] et construit par Harper [4] est devenu un outil précieux pour étudier ce problème. L'idée de remplacer le quasi-moment par la quantité de mouvement en mécanique quantique est le point crucial: $\hbar\mathbf{k} \to \boldsymbol{\pi}$, et nous verrons les détails dans la section suivante. Nous l'appelons aujourd'hui le modèle de Hofstadter, parce que Hofs-

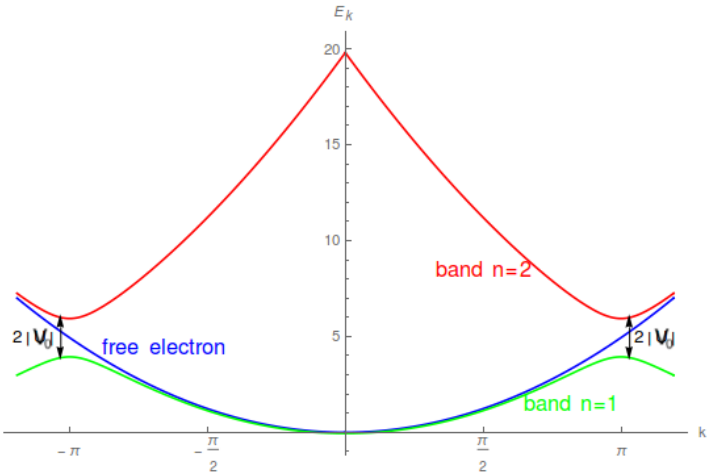

Figure 1: *Les bandes d'énergie des ondes de Bloch dans la première zone de Brillouin d'un système unidimensionnel: la courbe de dispersion d'énergie E_k vs. k avec le potential $V(x) = V_0 \sum_g e^{-igx}$ ($g = 2n\pi/a$, est le vecteur de réseau réciproque) avec $V_0 = -2$ (les courbes rouge et verte) et avec $V_0 = 0$ (la courbe bleue correspond à l'énergie de l'électron libre $E_k = \frac{\hbar^2 k^2}{2m}$). Poser: $a \to 1$,$\hbar \to 1$ et $m \to 1$. Les gaps à $k = \pm\pi$ sont les énergies interdites entre la première bande et la seconde bande, and they are equal to $2|V_0|$.*

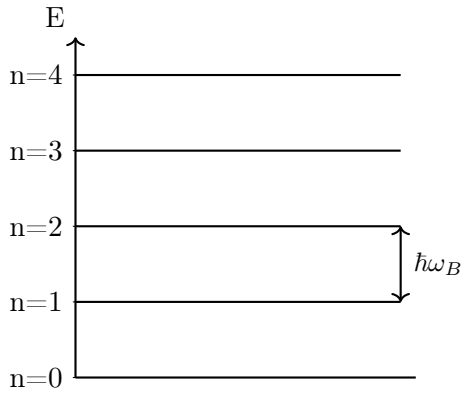

Figure 2: *Landau level: The degeneracy of the Landau level is infinite, $n \in \mathbb{N}$ is the index of energy level.*

tadter a été le premier à donner une image intuitive de son spectre fascinant. La figure fig. 1.3 représente le papillon de Hofstadter. Ce spectre fractal est le résultat de la compétition entre deux échelles de longueur: la longueur magnétique $l_B = \sqrt{\hbar/(eB)}$, et la paramètre cristallin a. Il affiche les énergies permises d'un électron par rapport au flux magnétique. Cette structure auto-similarité a une richesse mathématique et en même temps une signification physique: il est associé à l'effet Hall quantique entier, chaque intervalle d'énergie (la région vide du spectre) correspond à une quantification entière de la conductivité de Hall. De plus, le spectre lui-même a son propre intérêt mathématique pour les études liées à l'analyse spectrale. L'une des motivations de Hofstadter pour étudier ce problème réside dans les différentes caractéristiques du spectre pour les cas de champs magnétiques "rationnels" (quand le flux magnétique sur le flux quantique par unité de cellule est égal à p/q avec p et q sont premiers entre eux)

et de champs magnétiques "irrationnels" (lorsque le rapport entre les flux est irrationnel). Pour le cas "rationnel", la structure du spectre est constituée de q bandes, il est continu pour chaque bande et ne se chevauche jamais sauf si q est pair, alors les deux bandes centrales se touchent à l'énergie nulle. Pour le cas "irrationnel", le spectre se divise en un nombre infini de sous-bandes formant l' ensemble de Cantor de mesure nulle [5]. À l'époque de sa découverte, le papillon de Hofstadter avait plus d'intérêt théorique que de "vrais problèmes". Voici une citation de l'article original de Hofstadter [6] "The method is illustrated in a maximally simple model of the physical situation, but the ideas which arise are, it is to be hoped, applicable to more realistic models of the physical situation." Cependant, 40 ans plus tard, les physiciens ont trouvé des indications expérimentales sur ce spectre exotique. [7]. Maintenant, beaucoup de documents ont été publiés sur le papillon Hofstadter. Expérimentalement, il a découvert de nouveaux intérêts pour les atomes ultra-froids dans les réseaux optiques [8]. Théoriquement, des travaux récents, par exemple, montrent que le problème des valeurs propres quantiques des variétés de Calabi-Yau est étroitement lié au modèle de Hofstadter [9] (ne mentionnant même pas les nombres de Chern, la géométrie non commutative...). En tant que personnage émerveillé par le papillon de Hofstadter, j'espère convaincre le lecteur que même s'il jette un coup d'œil à lui, son charme ne faiblit jamais.

Le modèle de Hofstadter

Le modèle physique menant au papillon de Hofstadter est simple: une particule chargée se déplace sur un réseau carré couplé à un champ magnétique perpendiculaire. (fig. 1.4).On peut le considérer comme un tight-binding modèle dans lequel il existe une seule bande de Bloch lorsque le champ magnétique est appliqué [6], mais il pourrait aussi être compris comme un électron libre dans un champ magnétique homogène, et chaque niveau de Landau est divisé en sous-bandes par un potentiel périodique [10]. Ces deux approches alternatives conduisent au même spectre [11].

Dans cette thèse, je vais utiliser la présentation du tight-binding modèle, i.e. commencer par la fonction d'onde Bloch et ajouter le champ magnétique. Dans cette configuration, on suppose que l'électron se déplace sur un réseau carré avec le paramètre de réseau a et ne peut sauter que vers ses voisins les plus proches. Le tight-binding modèle est une méthode semi-empirique utilisée pour calculer la structure de la bande d'énergie et les états de Bloch à une seule particule d'un matériau. La philosophie ici est de supposer que les atomes dans un cristal sont localisés et séparés par une distance égale, le cristal est comme un réseau, et chaque site est un atome, la distance entre chaque atome est le paramètre de réseau. Par conséquent, l'électron dans un tel modèle est étroitement lié aux atomes, et sa fonction d'onde est approchée par une combinaison linéaire des orbitales atomiques situés à chaque site.

bande unique en réseau carré 2D

Le tight-binding modèle n'inclut pas les interactions électron-électron. L'Hamiltonien indépendant du temps à un seul électron est écrit

$$H = \sum_i \epsilon_i |i\rangle \langle i| + \sum_{\{i,j\}} t_{i,j} |i\rangle \langle j|$$

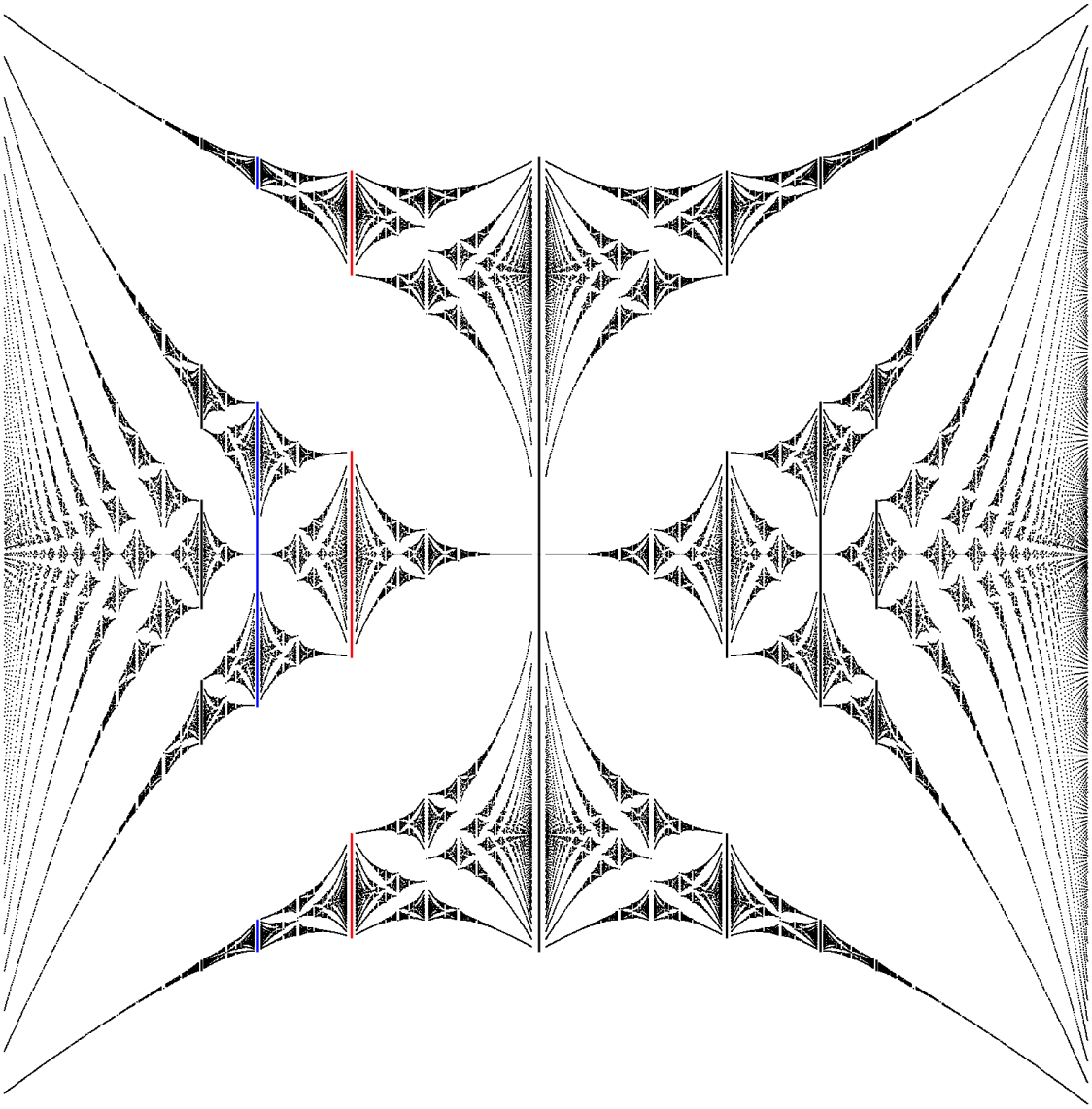

Figure 3: *Hofstadter's butterfly: Energy is plotted in unit*

où i désigne l'indice des sites sur un réseau et $\{i, j\}$ sont les voisins les plus proches et ϵ_i est l'énergie du site. Dans le modèle de liaison serré, la solution est développée en termes de orbitales atomiques. Soit $\phi_l(\mathbf{r} - \mathbf{R_j})$ le l-ème niveau atomique sur le site du réseau $\mathbf{R_j} = a(m_j\overrightarrow{e_x} + n_j\overrightarrow{e_y})$ où a est le paramètre de réseau, m_j et n_j sont des entiers. Par conséquent, la fonction d'onde de Bloch est

$$\psi_{\mathbf{k},l}(\mathbf{r}) = \sum_j e^{i\mathbf{k}\mathbf{R_j}} \sum_l \phi_l(\mathbf{r} - \mathbf{R_j})$$

Maintenant, considérons une seule bande, nous désignons l'état correspondant par $|s\rangle$ tel que $\langle \mathbf{r}|s\rangle = \phi(\mathbf{r} - \mathbf{R_s})$. Ainsi, la fonction d'onde de Bloch peut être réécrite comme suit: $\langle \mathbf{r}|\mathbf{k}\rangle$

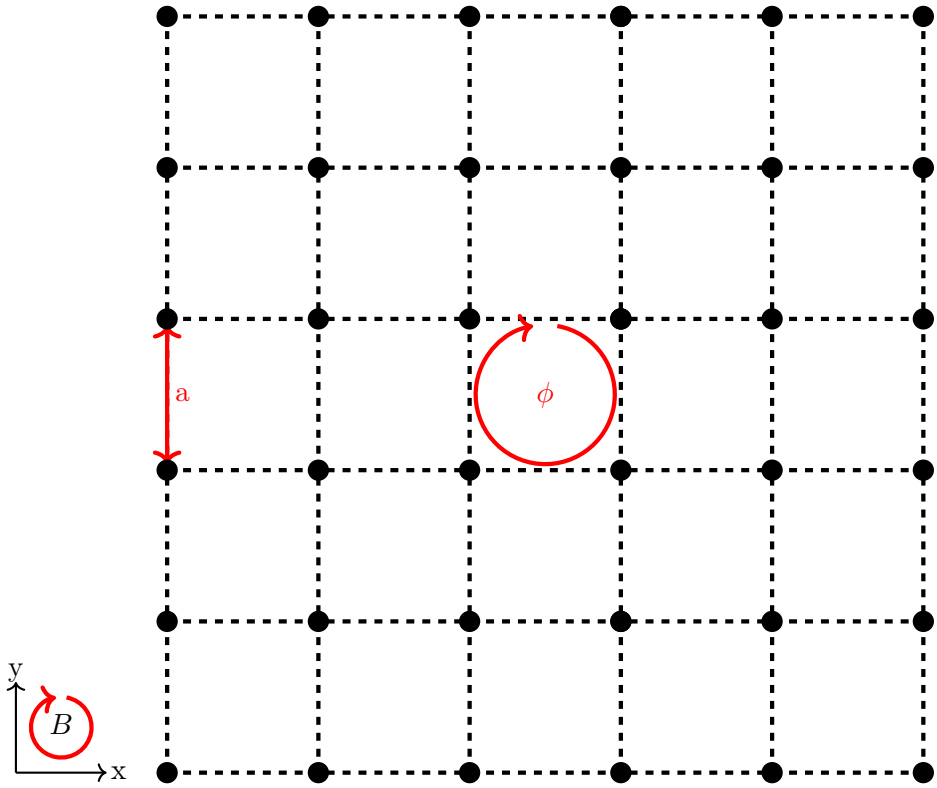

Figure 4: *un seul électron sautille entre les sites d'un réseau carré soumis à un champ magnétique perpendiculaire B: a est le paramètre d'espacement et $\phi = Ba^2$ représente le flux magnétique à travers une cellule unitaire*

avec $|\mathbf{k}\rangle = \sum_s e^{i\mathbf{k}\mathbf{R_s}}|s\rangle$. l'équation de valeur propre devient

$$E(k) = \frac{\langle \mathbf{k}|H|\mathbf{k}\rangle}{\langle \mathbf{k}|\mathbf{k}\rangle} = \epsilon_s + \sum_j t_{sj} e^{i\mathbf{k}(\mathbf{R_s}-\mathbf{R_j})}$$

où $\langle s|H|s\rangle = \epsilon_s$, $\langle s|H|j\rangle = t_{sj}$. En supposant $\epsilon_s = 0$ et $t_{sj} = t$ est non nul uniquement lorsque l'électron saute entre les sites les plus proches voisins ($|\mathbf{R_s} - \mathbf{R_j}| = a$), alors, on a

$$E = 2t\left(\cos(ak_x) + \cos(ak_y)\right)$$

Avec le Ansatz Onsager-Peierls: remplace $\hbar\boldsymbol{k}$ par $\boldsymbol{p}$:

$$\begin{aligned} E &= 2t\left(\cos(ap_x/\hbar) + \cos(ap_y/\hbar)\right) \\ &= t\left(e^{iap_x/\hbar} + e^{-iap_x/\hbar} + e^{iap_y/\hbar} + e^{-iap_y/\hbar}\right) \end{aligned}$$

où $p_x = -i\hbar\frac{\partial}{\partial x}$ et $p_y = -i\hbar\frac{\partial}{\partial y}$, alors

$$\epsilon = E/t = \left(T_x + T_x^{-1} + T_y + T_y^{-1}\right)$$

Sans le champ magnétique, T_x, T_y et leurs inverses ne sont que des opérateurs de translation dans chaque direction, tels que

$$T_x = e^{\frac{i}{\hbar}ap_x} \text{ and } T_y = e^{\frac{i}{\hbar}ap_y}.$$

Ils agissent sur un état $\Psi_{m,n}$ sur un site de réseau m, n comme suit

$$T_x^{\pm 1}\Psi_{ma,na} = \Psi_{(m\pm 1)a,na}$$
$$T_y^{\pm 1}\Psi_{ma,na} = \Psi_{ma,(n\pm 1)a}$$

Nous trouvons donc le

$$H = \left(T_x + T_x^{-1} + T_y + T_y^{-1}\right) \tag{1}$$

Cependant, lorsque le champ magnétique B est appliqué dans la direction z avec un vecteur potentiel $\boldsymbol{A}$, il rompt la symétrie de translation de l'Hamiltonien car le potentiel vectoriel $\boldsymbol{A}$ n'est pas invariant en déplaçant un vecteur de réseau. En utilisant la substitution de Peierls [3], on a remplacé l'opérateur momentum $\boldsymbol{p}$ par $\boldsymbol{p} - e\boldsymbol{A}/c$ (e étant la charge électrique élémentaire et c est la vitesse de la lumière). Par conséquent, en fonction du choix de jauge qu'on a fait, les opérateurs de translation doivent être multipliés par une phase supplémentaire. Dans cette thèse, nous travaillons avec le choix de jauge $\boldsymbol{A} = (0, Bx, 0)$ appelé jauge de Landau. Avec cette jauge, les opérateurs de translation dans x direction ne changent pas, les opérateurs de traduction dans y direction doivent se multiplier par une phase supplémentaire:

$$\begin{aligned} T_x^{\pm 1}\Psi_{ma,na} &= e^{\pm\frac{i}{\hbar}ap_x}\Psi_{ma,na} = \Psi_{(m\pm 1)a,na} \\ T_y^{\pm 1}\Psi_{ma,na} &= e^{\pm\frac{i}{\hbar}a(p_y - eBx/c)}\Psi_{ma,na} = e^{\mp\frac{i}{\hbar}aeBx/c}\Psi_{ma,(n\pm 1)a}. \end{aligned} \tag{2}$$

T_y et T_y^{-1} sont maintenant appelés les opérateurs de translation magnétique. En raison de la présence du champ magnétique, T_x et T_y avoir une structure non commutative:

$$T_x T_y = e^{-i\gamma} T_y T_x \tag{3}$$

où $\gamma = 2\pi\frac{\phi}{\phi_0}$, $\phi = Ba^2$ est le flux magnétique par unité de cellule de réseau, $\phi_0 = hc/e$ est le flux quantique. Dans ce qui suit, on a défini $a = 1$. La jauge de Landau brise l'invariance de translation dans le x direction, mais pas dans le y direction, on peut donc supposer le comportement de l'onde plane dans la direction y (les fonctions d'onde dans la direction y sont les états propres de p_y):

$$\Psi_{m,n} = e^{ink_y}\Phi_m \quad \text{and } k_y \text{ is the wave number in the } y \text{ direction}$$

En utilisant toutes les substitutions ci-dessus, on obtient une équation simplifiée à une différence propre unidimensionnelle

$$\Phi_{m+1} + \Phi_{m-1} + 2\cos(k_y + \gamma m)\Phi_m = E\Phi_m \tag{4}$$

où E est l'énergie. Cette équation s'appelle l'équation de Harper [4]. Dans le cas correspondant, quand γ est 'rationnel', i.e $\gamma = 2\pi\frac{p}{q}$ avec p et q sont des entiers co-prime, ce modèle simplifie considérablement. Nous allons nous concentrer sur ce cas dans ce qui suit.

Lien entre le modèle Hofstadter et les marches aléatoires

En 1997, en utilisant des techniques de géométrie non-commutative sur l'Hamiltonian de Hofstadter eq. (1.1), Bellissard et al ([12]) ont mis en relation la distribution en aire des

marches aléatoires fermées de longueur n avec le n-ième moment de l'Hamiltonien. Pour voir cette relation, nous définissons la fonction génératrice $Z_{m_1,m_2,l_1,l_2}(Q)$

$$Z_{m_1,m_2,l_1,l_2}(Q) = \sum_A C_{m_1,m_2,l_1,l_2}(A) Q^A \tag{5}$$

où $C_{m_1,m_2,l_1,l_2}(A)$ est le nombre de deux dimensions marches aléatoires sur un réseau carré avec m_1 nombre de pas vers la droite, m_2 nombre de pas vers la gauche, l_1 nombre de pas en haut et l_2 nombre de pas en bas, qui enferment une aire algébrique A. Pour les marches aléatoires fermées de longueur n, on définit

$$Z_n(Q) = \sum_{m=0}^{n/2} Z_{m,m,n/2-m,n/2-m}(Q) \tag{6}$$

où il y a $m_1 = m_2 = m$ pas dans la direction horizontale, et $l_1 = l_2 = n/2 - m$ pas dans la direction verticale. L'explication spécifique de ces notations est donnée dans le chapitre suivant.

Le processus de trouver la correspondance entre les marches aléatoires et le modèle Hofstadter est la suivante

- La trace par cellule unitaire est définie comme

  $$\text{Tr}\left(T_x^{n_1} T_y^{n_2}\right) = \delta_{n_1 \vec{x} + n_2 \vec{y},0} \tag{7}$$

  où n_1 et n_2 sont des entiers. Par exemple, $\text{Tr}\left(T_x T_x^{-1} T_y T_y^{-1}\right) = 1$, parceque $n_1 = n_2 = 0$ dans ce cas. T_x, T_y et leurs inverses sont des opérateurs de translation et ils sont définis comme eq. (1.2) .

- Selon eq. (1.1), l'Hamiltonian de Hofstadter élevé à la puissance de n est écrit comme

  $$H_\gamma^n = \left(T_x + T_x^{-1} + T_y + T_y^{-1}\right)^n$$

  Réécrire l'équation ci-dessus en utilisant la relation non commutative eq. (1.3), on trouve

  $$\left(T_x + T_x^{-1} + T_y + T_y^{-1}\right)^n = \sum_{\substack{m_1,m_2,l_1,l_2 \geq 0 \\ m_1+m_2+l_1+l_2=n}} Z_{m_1,m_2,l_1,l_2}\left(e^{i\gamma}\right) T_x^{m_1-m_2} T_y^{l_1-l_2} \tag{8}$$

  où $Z_{m_1,m_2,l_1,l_2}\left(e^{i\gamma}\right)$ est la fonction génératrice définie dans eq. (1.5) avec $Q = e^{i\gamma}$. Et comme mentionné précédemment, $\gamma = 2\pi\frac{\phi}{\phi_0}$, correspond au rapport entre le flux magnétique ϕ par cellule de réseau et le quantum de flux ϕ_0 . Par conséquent, quand $Q = e^{i\gamma}$, nous mappons les marches aléatoires classiques au modèle quantique de Hofstadter.

- Utilisant eq. (1.7) et eq. (1.8), le n-ième moment de l'Hamiltonian de Hofstadter est:

  $$\text{Tr}\, H_\gamma^n = \sum_{m=0}^{n/2} Z_{m,m,n/2-m,n/2-m}\left(e^{i\gamma}\right) = Z_n\left(e^{i\gamma}\right). \tag{9}$$

  L'opérateur de trace eq. (1.7) s'assure que cette somme n'est prise que sur des chemins fermés de longueur n. Donc, n devrait être pair.

L'équation eq. (1.9) relie le modèle quantique de Hofstadter aux chemins de réseau classiques. Comme mentionné précédemment, dans ce qui suit, nous nous concentrons sur le cas $\gamma = 2\pi\frac{p}{q}$ avec p et q sont des entiers co-prime. Dans le chapter 2, nous allons utiliser cette connexion en nous concentrant sur les marches aléatoires.

Contents

Chapter

1 Introduction

1.1 Overview and Motivations

In 1976, a paper about the energy levels of a single electron moving in a two-dimensional lattice coupled to a magnetic field was published. This paper plotted one of the first quantum fractals, known as the Hofstadter's butterfly (fig. 1.3), named after its discoverer, Douglas Hofstadter. However, the study of this model appeared much earlier. Felix Bloch [1] is the pioneer with one of the earliest contributions. In 1929, only five years after Erwin Schrödinger derived the Schrödinger equation, Bloch published a paper about the band structure of a single electron in a crystal lattice subjected to a periodic potential $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{T})$ (where the period $\mathbf{T} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}$ with n_1, n_2, n_3 are integers and $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ are the fundamental lattice vectors). Its Hamiltonian is $H = \frac{\mathbf{p}^2(\mathbf{r})}{2m} + V(\mathbf{r})$. Bloch's theorem states that the wavefunction of such an electron can be written as $\psi_{\boldsymbol{k},n}(\mathbf{r}) = u_{\boldsymbol{k},n}(\boldsymbol{r})e^{i\boldsymbol{kr}}$, where $\boldsymbol{k}$ is the wavevector and $u_{\boldsymbol{k},n}(\boldsymbol{r} + \boldsymbol{T}) = u_{\boldsymbol{k},n}(\boldsymbol{T})$ is a periodic function with the same periodicity as the potential $V(\mathbf{r})$. By using the Bloch wave function and the Fourier transformation, one can solve the eigenvalue function $H\psi_{\boldsymbol{k},n} = E_n(\boldsymbol{k})\psi_{\boldsymbol{k},n}$ (n is the band index). It turns out the energy spectrum of the Bloch wave function is not continuous, in fact, the presence of the lattice (periodic potential) breaks the energy (kinetic energy of free electron) into pieces. Each piece is called an energy band and the gaps between them are forbidden energy regions (see fig. 1.1, the simplest case: mixing of the first two bands only).

On the other hand, almost in the same period, Landau [2] was working on the quantum model of a free electron under a perpendicular magnetic field $\mathbf{B}$ with Hamiltonian $H = \frac{(\mathbf{p}-e\mathbf{A}/\hbar)^2}{2m}$. One can introduce $\boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}/\hbar$ with the commutation relation $[\pi_x, \pi_y] = ie\hbar B$, and define the operators $a = \frac{1}{2e\hbar B}(\pi_x - i\pi_y)$ and $a^+ = \frac{1}{2e\hbar B}(\pi_x + i\pi_y)$ with $[a, a^+] = 1$. a and a^+ are similar to the raising and lowering operators of an harmonic oscillator. By using the substitutions above, the Hamiltonian becomes $H = \frac{\boldsymbol{\pi}^2}{2m} = \hbar\omega_B(a^+a + \frac{1}{2})$ with $\omega_B = eB/m$ the cyclotron frequency. The quantized eigenenergies are now known as the Landau levels: $E_n = \hbar\omega_B(n + 1/2)$ where n is the Landau level index with an infinite degeneracy equals to the flux of the magnetic field in unit of the flux quantum. Thus, in the presence of an uniform magnetic field, the energies are evenly spaced, and the gap between each level is proportional to the magnetic field (see fig. 1.2).

The natural question is to combine these two problems: what will happen if someone puts an electron on a discrete lattice and then applies a perpendicular magnetic field to it? Lots of physicists have been interested in this problem over decades. Among them, a simple model conceived by Onsager and Peierls [3] and built by Harper [4] became a valuable tool to study this problem. The idea to replace the crystal momentum with the quantum mechanics momentum operator is the crucial point: $\hbar\mathbf{k} \to \boldsymbol{\pi}$, and we will see the details in the next section. Today we call it the Hofstadter's model because Hofstadter was the

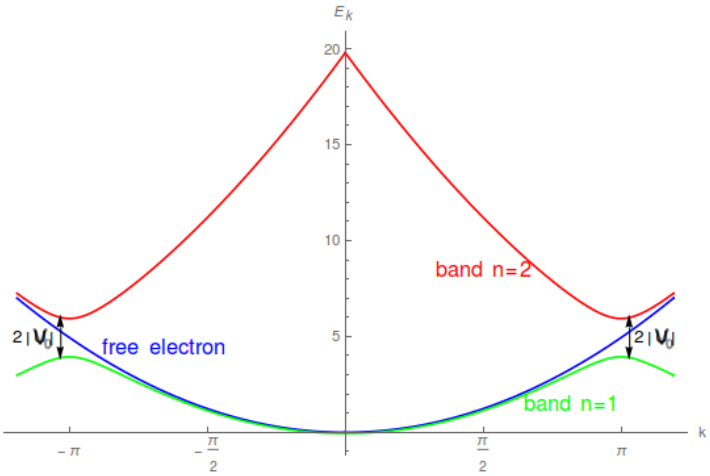

Figure 1.1: *Bloch wave bands in the first Brillouin zone in a one-dimensional system: the energy dispersion curve of E_k vs. k with the potential $V(x) = V_0 \sum_g e^{-igx}$ ($g = 2n\pi/a$, is the reciprocal lattice vector) with $V_0 = -2$ (red and green curve) and with $V_0 = 0$ (blue curve corresponds to the energy of free electron $E_k = \frac{\hbar^2 k^2}{2m}$). Set: $a \to 1$,$\hbar \to 1$ and $m \to 1$. The gaps at $k = \pm\pi$ are the energy gaps between the first band and the second band, and they are equal to $2|V_0|$.*

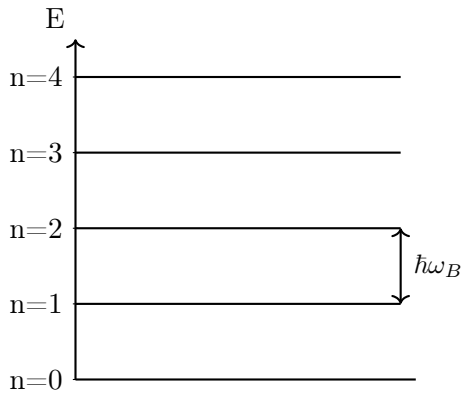

Figure 1.2: *Landau level: The degeneracy of the Landau level is infinite, $n \in \mathbb{N}$ is the index of energy level.*

first to give an intuitive picture for its fascinating spectrum. The figure fig. 1.3 represents the Hofstadter butterfly. This fractal spectrum is the result of the competition between two length scales: the magnetic length $l_B = \sqrt{\hbar/(eB)}$, and the lattice parameter a. It displays the allowed energies of an electron versus the magnetic flux. This self-similarity structure has a mathematically richness and at the same time a physical meaning: it is associated to the quantum Hall effect, each energy gap (the empty region in the spectrum) corresponds to an integer quantification of the Hall conductivity. Moreover, the spectrum itself has its own mathematical interest for studies related to spectral analysis. One of the motivations for Hofstadter to study this problem is the different features of the spectrum for the cases "rational" magnetic fields (when the magnetic flux over the flux quantum per unit cell equals to p/q with p and q are coprimes) and "irrational" magnetic fields (when the ratio between the flux is irrational). For the "rational" case, the structure of the spectrum consists of q bands,

it is continuous for each band and never overlap unless q is even then the two central bands touch each other at zero energy. For the "irrational" case, the spectrum splits into an infinite number of subbands forming a zero measure Cantor set [5]. Back at the time of its discovery, Hofstadter's butterfly had more theoretical interest than related to "real problems". Here is a quote from Hofstadter's original paper [6] "The method is illustrated in a maximally simple model of the physical situation, but the ideas which arise are, it is to be hoped, applicable to more realistic models of the physical situation." However, 40 years later, physicists have found experimental indications of this exotic spectrum [7]. Now lots of papers have been published about the Hofstadter butterfly. Experimentally, it has found some new interests for ultracold atoms in optical lattices [8]. Theoretically, some recent work, for example, shows that the quantum eigenvalues problem of Calabi-Yau manifolds is closely related to the Hofstadter model [9] (not even mentioning Chern numbers, non-commutative geometry...). Being one of the people who was amazed by Hofstatder's butterfly, I hope to convince the reader that even if he just takes a glimpse of it, its charm never decays.

1.2 The Hofstadter model

The physical model leading to the Hofstadter's butterfly is simple: a single particle moving on a two-dimensional lattice coupled to a magnetic field perpendicular to the lattice (fig. 1.4). One can consider it as a tight-binding model in which there is a single Bloch band when the magnetic field is applied [6], but it could also be understood as a free electron in a uniform magnetic field, and each single Landau level is split into subbands by a periodic potential [10]. These two alternative approaches lead to the same spectrum [11].

In this thesis, I will use the tight binding model presentation, i.e. start with the Bloch wave function and add the magnetic field. Under this configuration, we assume that the electron moves on a square lattice with lattice parameter a and can only jump to its nearest-neighbors. The tight binding model is a semi-empirical method used to calculate the energy band structure and the single-particle Bloch states of a material. The philosophy here is assuming that the atoms in a crystal are localized and separated by equal distance, the crystal is like a lattice, and each site is an atom, the distance between each atom is the lattice parameter. Therefore the electron in such a model is tightly bound to the atoms, and its wave function is approximated by a linear combination of atomic orbitals located at each site.

single band in 2D square lattice

The tight binding model does not include electron-electron interactions. The single electron time-independent Hamiltonian is written as

$$H = \sum_i \epsilon_i |i\rangle \langle i| + \sum_{\{i,j\}} t_{i,j} |i\rangle \langle j|$$

where i denotes the index of sites on a lattice and $\{i, j\}$ are the nearest neighbors and ϵ_i is the site energy. In the tight binding model, the solution is expanded in terms of atomic orbitals. Let $\phi_l(\mathbf{r} - \mathbf{R_j})$ be the l-th atomic level at the lattice site $\mathbf{R_j} = a(m_j\overrightarrow{e_x} + n_j\overrightarrow{e_y})$ where a is the lattice parameter, m_j and n_j are integers. Therefore the Bloch wavefunction is

$$\psi_{\mathbf{k},l}(\mathbf{r}) = \sum_j e^{i\mathbf{k}\mathbf{R_j}} \sum_l \phi_l(\mathbf{r} - \mathbf{R_j})$$

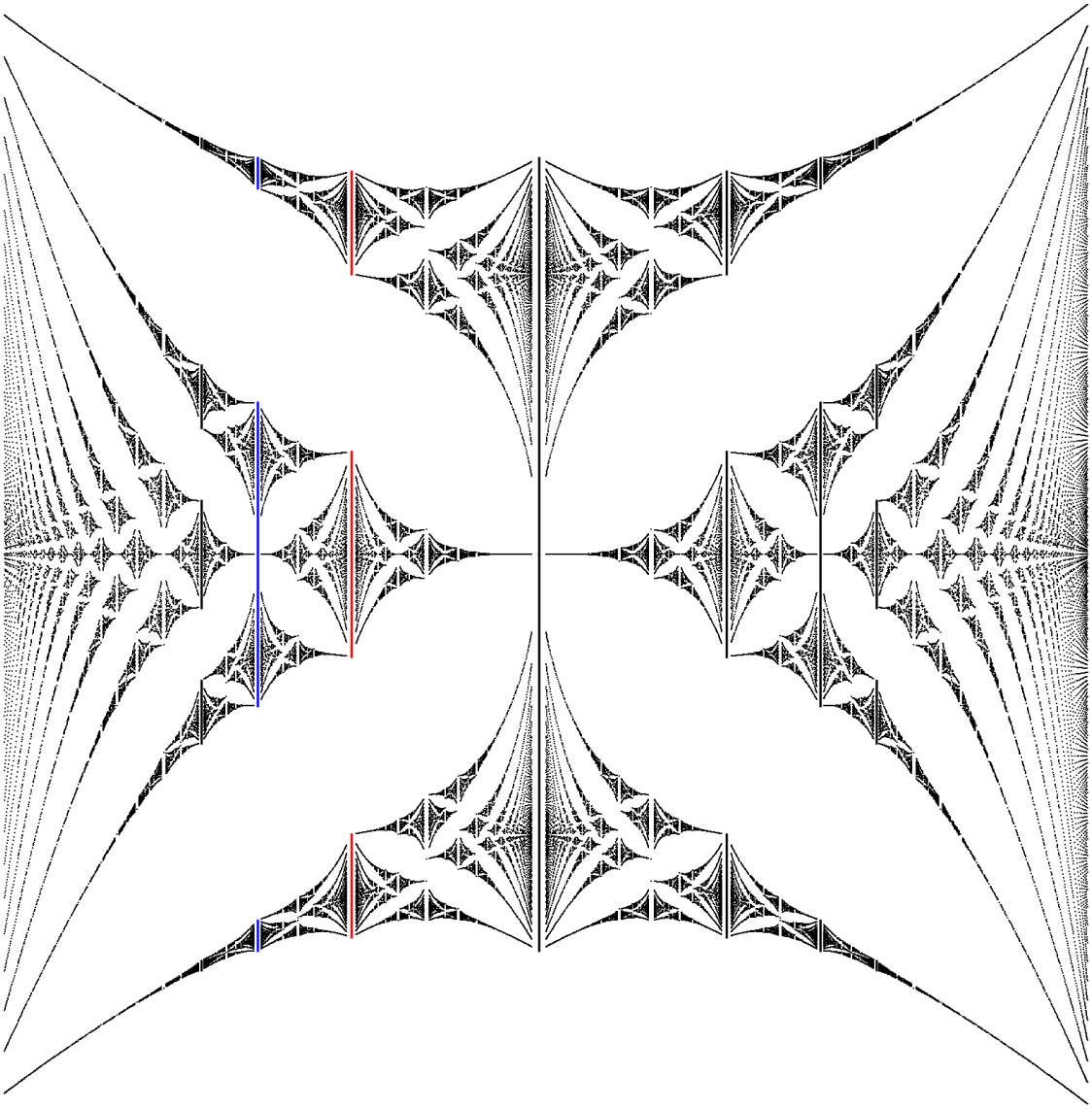

Figure 1.3: *Hofstadter's butterfly: Energy is plotted in unit*

Now, consider a single band, we denote the corresponding state by $|s\rangle$ such that $\langle \mathbf{r}|s\rangle = \phi(\mathbf{r} - \mathbf{R_s})$. Thus, the Bloch wavefunction can be rewritten as $\langle \mathbf{r}|\mathbf{k}\rangle$ with $|\mathbf{k}\rangle = \sum_s e^{i\mathbf{k}\mathbf{R_s}}|s\rangle$. the eigenvalue equation becomes

$$E(k) = \frac{\langle \mathbf{k}|H|\mathbf{k}\rangle}{\langle \mathbf{k}|\mathbf{k}\rangle} = \epsilon_s + \sum_j t_{sj} e^{i\mathbf{k}(\mathbf{R_s}-\mathbf{R_j})}$$

where $\langle s|H|s\rangle = \epsilon_s$, $\langle s|H|j\rangle = t_{sj}$. Assuming $\epsilon_s = 0$ and $t_{sj} = t$ is nonzero only when the electron is hopping between the nearest-neighbor sites ($|\mathbf{R_s} - \mathbf{R_j}| = a$), then we get

$$E = 2t\left(\cos(ak_x) + \cos(ak_y)\right)$$

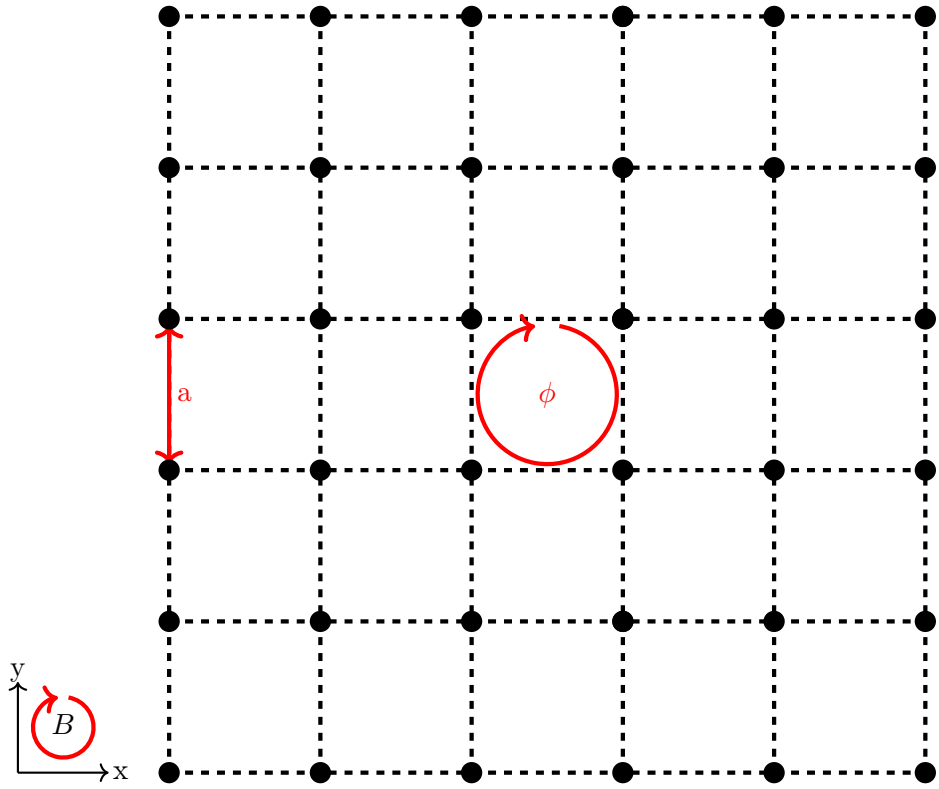

Figure 1.4: *a single electron hops between sites in a square lattice subjected to a perpendicular magnetic field B: a is the spacing parameter and $\phi = Ba^2$ represents the magnetic flux through a unit cell*

With the Onsager-Peierls Ansatz : replace $\hbar\boldsymbol{k}$ by $\boldsymbol{p}$:

$$\begin{aligned} E &= 2t\left(\cos(ap_x/\hbar) + \cos(ap_y/\hbar)\right) \\ &= t\left(e^{iap_x/\hbar} + e^{-iap_x/\hbar} + e^{iap_y/\hbar} + e^{-iap_y/\hbar}\right) \end{aligned}$$

where $p_x = -i\hbar\frac{\partial}{\partial x}$ and $p_y = -i\hbar\frac{\partial}{\partial y}$, thus

$$\epsilon = E/t = \left(T_x + T_x^{-1} + T_y + T_y^{-1}\right)$$

Without the magnetic field, T_x, T_y and their inverses are just translation operators in each direction, such that

$$T_x = e^{\frac{i}{\hbar}ap_x} \text{ and } T_y = e^{\frac{i}{\hbar}ap_y}.$$

They act on a state $\Psi_{m,n}$ at a lattice site m, n as follows

$$\begin{aligned} T_x^{\pm 1}\Psi_{ma,na} &= \Psi_{(m\pm 1)a,na} \\ T_y^{\pm 1}\Psi_{ma,na} &= \Psi_{ma,(n\pm 1)a} \end{aligned}$$

Therefore we find the

$$H = \left(T_x + T_x^{-1} + T_y + T_y^{-1}\right) \tag{1.1}$$

However, when the magnetic field B is applied in the z direction with a vector potential $\boldsymbol{A}$, it breaks the translational symmetry of the Hamiltonian because the vector potential $\boldsymbol{A}$ is not invariant by shifting one lattice vector. By using the Peierls substitution [3], we replaced the momentum operator $\boldsymbol{p}$ by $\boldsymbol{p} - e\boldsymbol{A}/c$ (e being the elementary electric charge and c is the speed of light). Hence, depending on the gauge choice we made, the translation operators must be multiplied by an additional phase. In this thesis, we work with the gauge choice $\boldsymbol{A} = (0, Bx, 0)$ which is called the Landau gauge. With this gauge, the translation operators in x direction do not change, the translation operators in y direction must multiply by an additional phase:

$$\begin{aligned} T_x^{\pm 1}\Psi_{ma,na} &= e^{\pm\frac{i}{\hbar}ap_x}\Psi_{ma,na} = \Psi_{(m\pm 1)a,na} \\ T_y^{\pm 1}\Psi_{ma,na} &= e^{\pm\frac{i}{\hbar}a(p_y - eBx/c)}\Psi_{ma,na} = e^{\mp\frac{i}{\hbar}aeBx/c}\Psi_{ma,(n\pm 1)a}. \end{aligned} \tag{1.2}$$

T_y and T_y^{-1} are now called the magnetic translation operators. Because of the presence of the magnetic field, T_x and T_y have a non-commutative structure:

$$T_x T_y = e^{-i\gamma} T_y T_x \tag{1.3}$$

where $\gamma = 2\pi\frac{\phi}{\phi_0}$, $\phi = Ba^2$ is the magnetic flux per unit cell of lattice, $\phi_0 = hc/e$ is the quantum flux. In the following, we set $a = 1$. Landau gauge breaks the translational invariance in the x direction but not in the y direction, so we can assume the plane wave behavior in the y direction (wave functions in the y direction are the eigenstates of p_y):

$$\Psi_{m,n} = e^{ink_y}\Phi_m \quad \text{and } k_y \text{ is the wave number in the } y \text{ direction}$$

By using all the substitutions above, one gets a simplified one-dimensional difference eigenvalue equation

$$\Phi_{m+1} + \Phi_{m-1} + 2\cos(k_y + \gamma m)\Phi_m = E\Phi_m \tag{1.4}$$

where E is the energy. This equation is called the Harper's equation [4]. In the commensurate case, when γ is 'rational', i.e $\gamma = 2\pi\frac{p}{q}$ with p and q are co-prime integers, this model simplify considerably. We shall focus on this case in the following.

1.3 Connection between the Hofstadter model and random walks

In 1997, by using non-commutative geometry techniques on the Hofstadter Hamiltonian eq. (1.1), Bellissard et al ([12]) related the area distribution of closed random walks of length n to the n-th moment of the Hamiltonian. In order to see this relation, we define the generating function $Z_{m_1,m_2,l_1,l_2}(Q)$

$$Z_{m_1,m_2,l_1,l_2}(Q) = \sum_A C_{m_1,m_2,l_1,l_2}(A)Q^A \tag{1.5}$$

where $C_{m_1,m_2,l_1,l_2}(A)$ is the number of two-dimensional random walks on a square lattice with m_1 steps right, m_2 steps left, l_1 steps up and l_2 steps down, which enclose an algebraic area A. For closed random walks of length n, we define

$$Z_n(Q) = \sum_{m=0}^{n/2} Z_{m,m,n/2-m,n/2-m}(Q) \tag{1.6}$$

where there are $m_1 = m_2 = m$ steps in the horizontal direction, and $l_1 = l_2 = n/2 - m$ steps in the vertical direction. The specific explanation of these notations are given in the next chapter.

The process of finding the mapping between random walks and the Hofstadter model is as follows

- The trace per unit cell is defined as

$$\text{Tr } \left(T_x^{n_1} T_y^{n_2}\right) = \delta_{n_1 \vec{x} + n_2 \vec{y}, 0} \tag{1.7}$$

  where n_1 and n_2 are integers. For example, $\text{Tr}\left(T_x T_x^{-1} T_y T_y^{-1}\right) = 1$, because $n_1 = n_2 = 0$ in this case. T_x, T_y and their inverses are translation operators and they are defined as eq. (1.2) .

- From eq. (1.1) , the Hofstadter Hamiltonian raised to the power of n is written as:

$$H_\gamma^n = \left(T_x + T_x^{-1} + T_y + T_y^{-1}\right)^n$$

  Rewrite the equation above by using the noncommutative relation eq. (1.3), one gets

$$\left(T_x + T_x^{-1} + T_y + T_y^{-1}\right)^n = \sum_{\substack{m_1, m_2, l_1, l_2 \geq 0 \\ m_1 + m_2 + l_1 + l_2 = n}} Z_{m_1, m_2, l_1, l_2}\left(e^{i\gamma}\right) T_x^{m_1 - m_2} T_y^{l_1 - l_2} \tag{1.8}$$

  where $Z_{m_1, m_2, l_1, l_2}\left(e^{i\gamma}\right)$ is the generating function defined in eq. (1.5) with $Q = e^{i\gamma}$. And as mentioned before, $\gamma = 2\pi \frac{\phi}{\phi_0}$, corresponds to the ratio between the magnetic flux ϕ per unit lattice cell and the flux quantum ϕ_0 . Therefore, when $Q = e^{i\gamma}$, we map the classical random walks to the quantum Hofstadter model.

- Using eq. (1.7) and eq. (1.8) , the n-th moment of the Hofstadter Hamiltonian is:

$$\text{Tr } H_\gamma^n = \sum_{m=0}^{n/2} Z_{m, m, n/2-m, n/2-m}\left(e^{i\gamma}\right) = Z_n\left(e^{i\gamma}\right). \tag{1.9}$$

  The trace operator eq. (1.7) makes sure that this sum is only taken on closed paths of length n. Thus, n should be even.

Equation eq. (1.9) links the quantum Hofstadter model to classical lattice paths. As mentioned before, in the following, we focus on the case $\gamma = 2\pi \frac{p}{q}$ with p and q are co-prime integers. In chapter 2, we are going to use this connection by focusing on the random walks.

Chapter

2 The generating function $Z_{m_1,m_2,l_1,l_2}(Q)$ for random walks

In this chapter, we are going to show how to derive a formula for $Z_n\left(e^{2i\pi p/q}\right)$ in eq. (1.9), the generating function for the algebraic area of random walks. The results are published in [13] which is the Article 1 inserted at the end of this chapter.

In section 2.1, we shall first introduce some basic information about two-dimensional random walks and their algebraic areas. Also, we will analyse more in detail the generating function of the algebraic area of random lattice walks and its connection with the Hofstadter model. Then, we will present a method for deriving an expression for the multivariate generating function $Z_{m_1,m_2,l_1,l_2}(Q)$, which yields simple explicit formulas in some special cases. This multivariate generating function is then specialized to the generating function of $Z_n\left(e^{2i\pi p/q}\right)$. This allows us to derive a closed expression for $Z_n\left(e^{2i\pi p/q}\right)$ and thus, thanks to eq. (1.9), for the traces $\mathrm{Tr}\, H^n_{2\pi p/q}$, in terms of the Kreft coefficients eq. (2.18). We will also study the asymptotic behavior of $Z_n\left(e^{2i\pi p/q}\right)$ as $n \to \infty$ for a fixed $2\pi p/q$.

2.1 Random walks and their algebraic areas

The random walks we are talking about here are simple planar paths on a square lattice, made of a sequence of random steps with constant length taken into the four directions (up, down, left and right) with equal probability [14]. Therefore we define it as an ordered sequence of four basic steps: x denotes a step to the right, x^{-1} a step to the left, y a step up and y^{-1} a step down; m_1, m_2, l_1 and l_2 are the numbers of steps in these directions respectively. If e.g. a random walk has n steps, it is defined by a sequence $\{s_1, s_2, \ldots, s_n\}$, where each s_k with $k = 1, 2, \ldots, n$ can be one of the four operators $\{x, x^{-1}, y, y^{-1}\}$. Also, we label them such that s_i is the i-th step. A random walk is closed if and only if $m_1 = m_2 = m$ and $l_1 = l_2 = l$, i.e. a walk with an equal number of steps m in horizontal directions and an equal number of steps l in vertical directions. If its total length is n, then $m \in \{0, 1, \ldots, n/2\}$ and $l = n/2 - m$. Closed random walks on a square lattice enclose an algebraic area which is the number of square units surrounded by the walks. If the curve enclosed by random walks winds around more than once, the area is counted with multiplicity. The algebraic area is negative if the walk moves around clockwise, it is positive if the walk moves oppositely. If a walk is open, in order to define its algebraic area, we can close it by adding the necessary steps to connect its ending point with its starting point: we choose to add first the minimum necessary number of steps in vertical directions, then in horizontal directions. E.g., if an open lattice walk has

m_1 steps right, m_2 steps left, l_1 steps up and l_2 steps down, we add first $|l_1 - l_2|$ steps in the vertical direction then $|m_1 - m_2|$ steps in the horizontal direction in order to close it (see the illustration fig. 2.1 below). The total number of such random walks is

$$\binom{m_1 + m_2 + l_1 + l_2}{m_1, m_2, l_1, l_2}$$

The total number of closed paths with length n is thus

$$\sum_{m=0}^{n/2} \binom{n}{m, m, n/2 - m, n/2 - m} = \binom{n}{n/2}^2 \tag{2.1}$$

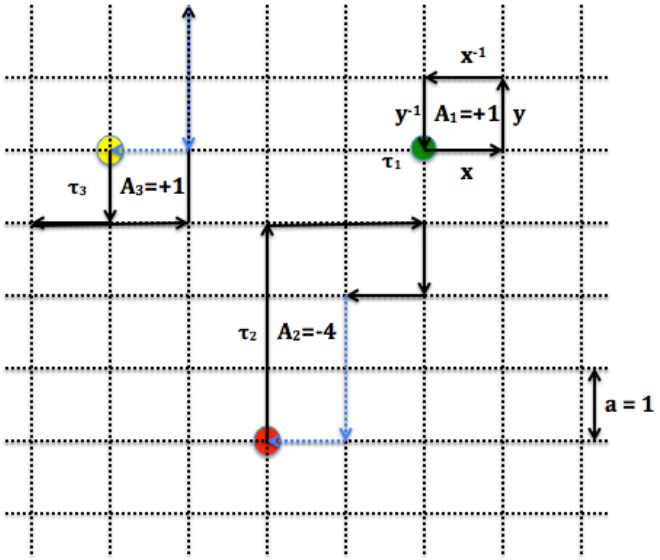

Figure 2.1: *Lattice parameter $a = 1$. Here are examples of 3 random walks and their algebraic area: τ_1 is a closed walk of 4 steps: it starts from the green point, first go right, next go up, then go left and finally go down to come back to its starting point. It turns like anticlockwise, and it enclosed one square unit, so its algebraic area is 1; τ_2 and τ_3 are two open walks of 7 steps, as explained above, we add first necessary vertical steps then horizontal steps to close them, and their algebraic areas are the number of square units enclosed by them with opposite signs because they move in opposite ways.*

Q-binomial theorem

Two random walks with the same number $\{m_1, m_2, l_1, l_2\}$ of steps in each direction are different if they have different order in their steps. In order to calculate the algebraic area A for $\{m_1, m_2, l_1, l_2\}$ given, we introduce a Q-commutator such that $xy = Qyx$. Multiplying both sides by x^{-1} and y^{-1} on the left and right, we get the full commutation relations between the four operators x, x^{-1}, y, y^{-1}

$$xy = Qyx; \quad yx^{-1} = Qx^{-1}y; \quad y^{-1}x = Qxy^{-1}. \tag{2.2}$$

By using the noncommutative relations eq. (2.2) , the algebraic area A of a closed random walk with n steps can be computed directly from the product of the sequence of steps $\{s_1, s_2, \ldots, s_n\}$

$$s_1 \cdots s_n = Q^A \mathbb{1}$$

where $s_k \in \{x, x^{-1}, y, y^{-1}\}$ with $k = 1, 2 \ldots, n$ as mentioned before. $\mathbb{1}$ represents the product of a normally ordered walk as

$$\{y^{-1}, y^{-1}, \ldots, y^{-1}, y, y, \ldots, y, x, x, \ldots, x, x^{-1}, x^{-1}, \ldots, x\}$$

where there are equal numbers of x and x^{-1}, and the same holds for y and y^{-1}. Such a walk obviously has zero algebraic area. Hence, the question of calculating the algebraic area of a closed random walk can be solved in three steps:

- First rearranging the sequence of the steps such that it is normally ordered;
- Then calculating the product of the sequence after the rearrange by using the noncommutative relations eq. (2.2);
- Finally summing up all the exponent of Q, which is the algebraic area A.

E.g., the closed lattice path τ_1 in fig. 2.1, its sequence of steps is $\{x, y, x^{-1}, y^{-1}\}$, so the product of this sequence is $xyx^{-1}y^{-1} = Qyxx^{-1}y^{-1} = Q$, the exponent of Q is one, and its algebraic area is indeed one. For the open walk τ_2 in fig. 2.1, its sequence of steps after closing is $\{y, y, y, x, x, y^{-1}, x^{-1}, y^{-1}, y^{-1}, x^{-1}\}$, the product of its sequence is $y^3x^2y^{-1}x^{-1}y^{-2}x^{-1} = Q^{-6}x^2y^2x^{-1}y^{-2}x^{-1} = Q^{-6+2}x^2x^{-1}y^{-2}y^2x^{-1} = Q^{-4}$, and its algebraic area is indeed -4. The other open path τ_3 in fig. 2.1, its sequence of steps after closing is $\{y^{-1}, x^{-1}, x, x, y, y, y, y^{-1}, y^{-1}, x^{-1}\}$, its product equals $y^{-1}xyx^{-1} = Qy^{-1}yxx^{-1} = Q$, the exponent of Q is one and its algebraic area is one.

If x and y satisfy $xy = Qyx$, then

$$(x + y)^n = \sum_{k=0}^{n} Z_{n,k}(Q) y^k x^{n-k}$$

where $Z_{n,k}(Q)$ is the Q-binomial coefficient:

$$Z_{n,k}(Q) = \binom{n}{k}_Q = \frac{[n]_Q!}{[k]_Q![n-k]_Q!} \tag{2.3}$$

with

$$[k]_Q! = 1(1+Q)(1+Q+Q^2)\cdots(1+Q+Q^2+\ldots+Q^{k-1}) = \prod_{i=1}^{k} \frac{1-Q^i}{1-Q}$$

when $Q = 1$, $[k]_Q!$ turns back into $k!$, the factorial of k and $Z_{n,k}(1)$ is the usual binomial coefficient $\binom{n}{k}$. We can understand $Z_{n,k}(Q)$ in the context of random walks: let x and y be the two unit operators which construct the "staircase walks", i.e. walks only go up and right. Thus, $Z_{n,k}(Q)$ is the generating function for the algebraic area distribution of the "staircase walks" with k right steps and $n-k$ up steps: $Z_{n,k}(Q) = \sum_A C_{n,k}(A)Q^A$ with $C_{n,k}(A)$ is the number of such walks enclosing an algebraic A. When $Q = 1$, $Z_{n,k}(1)$ is the number of such "staircase walks".

Generating function of the algebraic area

Let us recall the definitions in section 1.3 of chapter 1: $C_{m_1,m_2,l_1,l_2}(A)$ is the number of random walks which enclose an algebraic area A and have m_1 steps right, m_2 steps left, l_1 steps up and l_2 steps down. In order to study the algebraic area distribution of random walks, we use eq. (1.5), the generating function of the $C_{m_1,m_2,l_1,l_2}(A)$'s:

$$Z_{m_1,m_2,l_1,l_2}(Q) = \sum_{A=-A_-}^{A_+} C_{m_1,m_2,l_1,l_2}(A) Q^A \tag{2.4}$$

where $A_\pm$ is the maximum algebraic area enclosed by a path with $\{m_1, m_2, l_1, l_2\}$ steps.

$$A_\pm = \max(m_1, m_2)\max(l_1, l_2) - \frac{|(m_1 - m_2)(l_1 - l_2)| \pm (m_1 - m_2)(l_1 - l_2)}{2} \tag{2.5}$$

(A_+ is the maximum area covered in the positive direction (anticlockwise), A_- is the maximum area covered in the negative direction (clockwise)). In order to close a open path, one must first add the vertical necessary steps $|l_1 - l_2|$, then add the horizontal steps $|m_1 - m_2|$. Assuming that $m_1 > m_2$ and $l_1 > l_2$, then the ending point is at the top and right side of the initial point, thus, its maximum areas are $A_- = m_1 l_1$ and $A_+ = l_2 m_1 + l_1 m_2 - l_2 m_2$. The algebraic area probability distribution is given by

$$P_{m_1,m_2,l_1,l_2}(A) = \frac{C_{m_1,m_2,l_1,l_2}(A)}{\binom{m_1+m_2+l_1+l_2}{m_1,m_2,l_1,l_2}}$$

where $\binom{m_1+m_2+l_1+l_2}{m_1,m_2,l_1,l_2}$ is the total number of random walks with m_1 steps right, m_2 steps left, l_1 steps up and l_2 steps down as mentioned before. Then,

$$\sum_A P_{m_1,m_2,l_1,l_2}(A) Q^A = \frac{Z_{m_1,m_2,l_1,l_2}(Q)}{Z_{m_1,m_2,l_1,l_2}(1)} \tag{2.6}$$

This generating function $Z_{m_1,m_2,l_1,l_2}(Q)$ can be considered as a generalization of the Q-binomial coefficient $Z_{n,k}(Q)$ eq. (2.3). Thus

$$\left(x + y + x^{-1} + y^{-1}\right)^n = \sum_{\substack{m_1,m_2,l_1,l_2 \geq 0 \\ m_1+m_2+l_1+l_2=n}} Z_{m_1,m_2,l_1,l_2}(Q) y^{-l_1} y^{l_2} x^{m_1} x^{-m_2} \tag{2.7}$$

Rewrite $\left(x + y + x^{-1} + y^{-1}\right)^n$ as $\left(x + y + x^{-1} + y^{-1}\right)\left(x + y + x^{-1} + y^{-1}\right)^{n-1}$ and expand it by using the noncommutative relations eq. (2.2), one gets

$$\begin{aligned}
\left(x + y + x^{-1} + y^{-1}\right)^n = & \sum_{\substack{m_1,m_2,l_1,l_2 \geq 0 \\ m_1+m_2+l_1+l_2=n}} Q^{-l_1+l_2} Z_{m_1-1,m_2,l_1,l_2}(Q) y^{-l_1} y^{l_2} x^{m_1} x^{-m_2} \\
& + \sum_{\substack{m_1,m_2,l_1,l_2 \geq 0 \\ m_1+m_2+l_1+l_2=n}} Z_{m_1,m_2,l_1,l_2-1}(Q) y^{-l_1} y^{l_2} x^{m_1} x^{-m_2} \\
& + \sum_{\substack{m_1,m_2,l_1,l_2 \geq 0 \\ m_1+m_2+l_1+l_2=n}} Q^{l_1-l_2} Z_{m_1,m_2-1,l_1,l_2}(Q) y^{-l_1} y^{l_2} x^{m_1} x^{-m_2} \\
& + \sum_{\substack{m_1,m_2,l_1,l_2 \geq 0 \\ m_1+m_2+l_1+l_2=n}} Z_{m_1,m_2,l_1-1,l_2}(Q) y^{-l_1} y^{l_2} x^{m_1} x^{-m_2}
\end{aligned}$$

From above, it is easy to see that $Z_{m_1,m_2,l_1,l_2}(Q)$ obeys the recurrence relation

$$\begin{aligned} Z_{m_1,m_2,l_1,l_2}(Q) = & Z_{m_1,m_2,l_1-1,l_2}(Q) + Z_{m_1,m_2,l_1,l_2-1}(Q) \\ & + Q^{l_2-l_1} Z_{m_1-1,m_2,l_1,l_2}(Q) + Q^{l_1-l_2} Z_{m_1,m_2-1,l_1,l_2}(Q) \end{aligned} \tag{2.8}$$

The physical interpretation of this recurrence relation is simply. For the random walks with m_1 right steps, m_2 left steps, l_1 up steps and l_2 down steps, we distinguish the four possible cases for the last step: if the last step is vertical, then the algebraic area does not change; If it is a step to the left, the algebraic area changes exactly by the current y-coordinate; the same holds if the last step is a step to the right, but with opposite sign (see fig. 2.2).

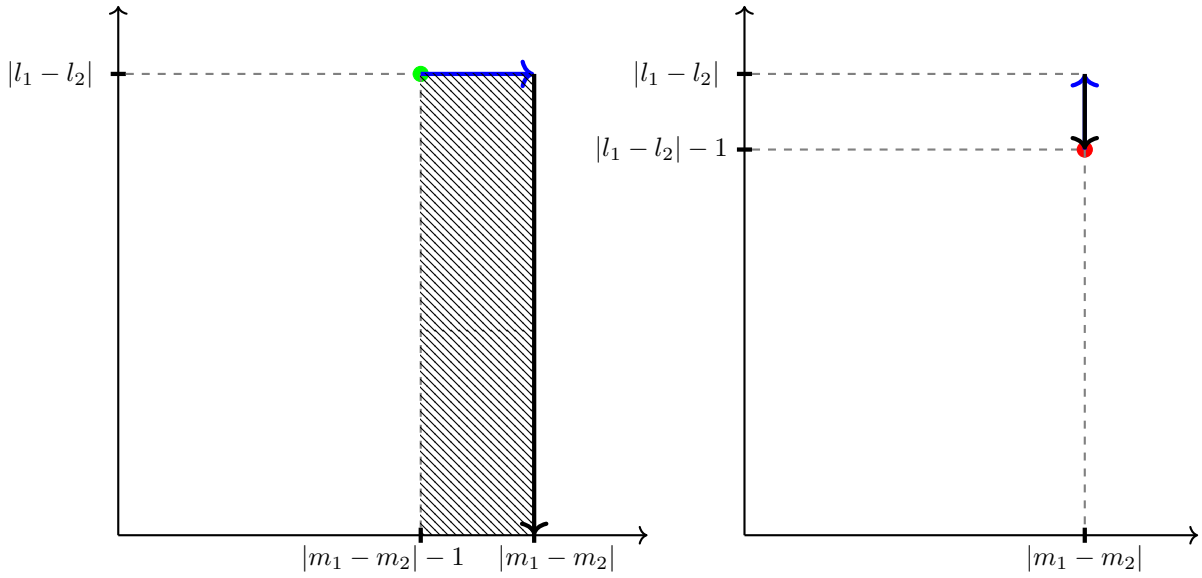

Figure 2.2: *two figures above are two cases for the last step of a path with* $\{m_1, m_2, l_1, l_2\}$ *steps (blue arrow represents the last step, and black arrow is used to close the path after the last step): the figure on the left corresponds to the last step goes right, its algebraic increases* $|l_1 - l_2|$ *in the negative direction(clockwise rotation); the figure on the right corresponds to the last step goes up, its algebraic area does not change.*

As mentioned in chapter 1, evaluate $Z_{m_1,m_2,l_1,l_2}(Q)$ at $Q = e^{i\gamma}$, and identify x, y (and their inverses) with the (magnetic) translation operators T_x and T_y (and their inverses), eq. (2.7) turns into eq. (1.8). By setting $Q = e^{i\gamma}$, we mapped classical random walks on the quantum Hofstadter model. Since we always focus on the case γ is rational, in the following, we will restrict to $Q = e^{2i\pi p/q}$ with p and q are coprime integers, which means Q is a q-th root of unity, so that $Q^q = 1$. In the next section.

2.2 The method for determining $Z_{m_1,m_2,l_1,l_2}(Q)$

In order to find an explicit formula for $Z_{m_1,m_2,l_1,l_2}(Q)$, we introduce the multivariate generating function

$$A(x_1,x_2,y_1,y_2,Q)=\sum_{m_1,m_2,l_1,l_2\geq 0} Z_{m_1,m_2,l_1,l_2}(Q)x_1^{m_1}x_2^{m_2}y_1^{l_1}y_2^{l_2}, \tag{2.9}$$

such that we can extract the information of $Z_{m_1,m_2,l_1,l_2}(Q)$ directly from its generating function $A(x_1,x_2,y_1,y_2,Q)$. By using the recurrence relation eq. (2.8) with the boundary conditions $Z_{0,0,0,0}(Q)=1$ and $Z_{m_1,m_2,l_1,l_2}(Q)=0$ when at least one of the $\{m_1,m_2,l_1,l_2\}$ is negative, one can read immediately

$$A(x_1,x_2,y_1,y_2,Q)=1+y_1A(x_1,x_2,y_1,y_2,Q)+y_2A(x_1,x_2,y_1,y_2,Q) \tag{2.10}$$

$$+x_1A(x_1,x_2,Q^{-1}y_1,Qy_2,Q)+x_2A(x_1,x_2,Qy_1,Q^{-1}y_2,Q). \tag{2.11}$$

Because $Q=e^{2i\pi p/q}$, is a root of unity, this turns into a finite system of linear equations. We set $A_k=A(x_1,x_2,Q^ky_1,Q^{-k}y_2,Q)$ with $A_0=A_q=A(x_1,x_2,y_1,y_2,Q)$. From eq. (2.10), we get

$$\begin{aligned}A_k&=A(x_1,x_2,Q^ky_1,Q^{-k}y_2,Q)\\&=1+Q^ky_1A(x_1,x_2,Q^ky_1,Q^{-k}y_2,Q)+Q^{-k}y_2A(x_1,x_2,Q^ky_1,Q^{-k}y_2,Q)\\&\quad+x_1A(x_1,x_2,Q^{k-1}y_1,Q^{-k+1}y_2,Q)+x_2A(x_1,x_2,Q^{k+1}y_1,Q^{-k-1}y_2,Q)\\&=1+(Q^ky_1+Q^{-k}y_2)A_k+x_1A_{k-1}+x_2A_{k+1}.\end{aligned}$$

This recurrence relation reduces to a matrix form

$$\begin{pmatrix} c_0 & -x_2 & 0 & \cdots & 0 & -x_1\\ -x_1 & c_1 & -x_2 & \cdots & 0 & 0\\ 0 & -x_1 & c_2 & \cdots & 0 & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & 0 & \cdots & c_{q-2} & -x_2\\ -x_2 & 0 & 0 & \cdots & -x_1 & c_{q-1}\end{pmatrix}\cdot\begin{pmatrix}A_0\\A_1\\A_2\\\vdots\\A_{q-2}\\A_{q-1}\end{pmatrix}=\begin{pmatrix}1\\1\\1\\\vdots\\1\\1\end{pmatrix},$$

where $c_k=1-Q^ky_1-Q^{-k}y_2$ and $Q=e^{2i\pi p/q}$. Then, we can use the Cramer's rule to solve $A(x_1,x_2,y_1,y_2,Q)$:

$$A(x_1,x_2,y_1,y_2,Q)=A_0=\frac{\begin{vmatrix}1 & -x_2 & 0 & \cdots & 0 & -x_1\\ 1 & c_1 & -x_2 & \cdots & 0 & 0\\ 1 & -x_1 & c_2 & \cdots & 0 & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 1 & 0 & 0 & \cdots & c_{q-2} & -x_2\\ 1 & 0 & 0 & \cdots & -x_1 & c_{q-1}\end{vmatrix}}{\begin{vmatrix} c_0 & -x_2 & 0 & \cdots & 0 & -x_1\\ -x_1 & c_1 & -x_2 & \cdots & 0 & 0\\ 0 & -x_1 & c_2 & \cdots & 0 & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & 0 & \cdots & c_{q-2} & -x_2\\ -x_2 & 0 & 0 & \cdots & -x_1 & c_{q-1}\end{vmatrix}} \tag{2.12}$$

where $c_k = 1 - Q^k y_1 - Q^{-k} y_2$ and $Q = e^{2i\pi p/q}$ as before. In order to see how this process works, In Article 1, we gave some simple examples with small values of q to show how to extract the explicit formula of $Z_{m_1,m_2,l_1,l_2}(Q)$ from its generating function $A(x_1, x_2, y_1, y_2, Q)$. Please also see the Appendix D for a complete derivation of $Z_{m_1,m_2,l_1,l_2}\left(e^{2i\pi/q}\right)$ in the case where $m_1 - m_2 \equiv l_1 - l_2 \equiv 0 \bmod q$ with $q = 3$ and $q = 4$ (we are particularly interested in this case because the closed random walk is a special situation of it: for closed random walks, $m_1 - m_2 = l_1 - l_2 = 0$.). In general, with the increase of q, the formula of $Z_{m_1,m_2,l_1,l_2}(Q)$ becomes more and more complicated. Fortunately, when Q is a root of unity, the generating function $A(x_1, x_2, y_1, y_2, Q)$ always has a general shape such that

$$A(x_1, x_2, y_1, y_2, Q) = \frac{U(x_1, x_2, y_1, y_2)}{1 - x_1^q - x_2^q - y_1^q - y_2^q + V(x_1 x_2, y_1 y_2)} \tag{2.13}$$

where U, V are polynomials and V is symmetric (in its two variables) and has only real coefficients (and constant coefficient 0). The section 3.3 of Article 1 shows how we obtained this general shape.

2.3 The generating function for closed random walks of length n : $Z_n(Q)$

As stated in the beginning, we want to calculate $Z_n(Q)$ in eq. (1.6), which corresponds to closed lattice walks of a given length n with $m_1 = m_2 = m$ and $l_1 = l_2 = n/2 - m$. This is simpler than the general case, because $\sum_{m=0}^{n/2} Z_{m,m,n/2-m,n/2-m}(Q)$ can be obtained directly from $A(x_1, x_2, y_1, y_2, Q)$ by setting $x_1 \to zx$, $x_2 \to z/x$, $y_1 \to zy$ and $y_2 \to z/y$ and looking at the coefficients of zero components of x and y and n component of z. Therefore the problem is reduced to two steps: first, finding the generating function for $Z_n(Q)$

$$\sum_{n\geq 0} Z_n(Q)\, z^n = [x^0 y^0] A(zx, z/x, zy, z/y, Q). \tag{2.14}$$

Then, expending $\sum_{n\geq 0} Z_n(Q)\, z^n$ and looking at the coefficients of z^n, that will give us the explicit formula of $Z_n(Q)$.

Now let us first focus on how to find the coefficient $[x^0 y^0] A(zx, z/x, zy, z/y, Q)$. From the eq. (2.12) and eq. (2.13), we have

$$A(zx, z/x, zy, z/y, Q) = \frac{U(zx, z/x, zy, z/y)}{1 - z^q\left(x^q + x^{-q} + y^q + y^{-q}\right) + V(z^2, z^2)} \tag{2.15}$$

The denominator of eq. (2.15) is the determinant of the $q \times q$ matrix

$$\Delta(zx, z/x, zy, z/y) = \begin{vmatrix} c_0 & -z/x & 0 & \cdots & 0 & -zx \\ -zx & c_1 & -z/x & \cdots & 0 & 0 \\ 0 & -zx & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} & -z/x \\ -z/x & 0 & 0 & \cdots & -zx & c_{q-1} \end{vmatrix}$$

where $c_k = 1 - Q^k zy - Q^{-k} z/y$ and $Q = e^{2i\pi p/q}$. Since $\Delta(zx, z/x, zy, z/y) = 1 - z^q\left(x^q + x^{-q} + y^q + y^{-q}\right) + V(z^2, z^2)$, this determinant is decomposed by two parts: one part is a polynomial of z

which is independent of x and y, we define it as $b_{p/q}(z) = 1 + V(z^2, z^2)$; the other part is $-z^q\,(x^q + x^{-q} + y^q + y^{-q})$. Thus, we have

$$b_{p/q}(z) = \Delta(z, z, z, z) + 4z^q$$

where $\Delta(z, z, z, z)$ is the determinant

$$\begin{vmatrix} 1-2z & -z & 0 & \cdots & 0 & -z \\ -z & 1-2z\cos\left(\frac{2\pi p}{q}\right) & -z & \cdots & 0 & 0 \\ 0 & -z & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & -z \\ -z & 0 & 0 & \cdots & -z & 1-2z\cos\left((q-1)\frac{2\pi p}{q}\right) \end{vmatrix}. \tag{2.16}$$

By computing this determinant, we get

$$b_{p/q}(z) = -\sum_{i=0}^{[q/2]} a_{p/q}(2i) z^{2i} \tag{2.17}$$

with coefficients $a_{p/q}(2i)$

$$a_{p/q}(2i) = (-1)^{i+1} \sum_{k_1=0}^{q-2i} \sum_{k_2=0}^{k_1} \cdots \sum_{k_i=0}^{k_{i-1}} 4\sin^2\left(\frac{\pi(k_1+2i-1)p}{q}\right) 4\sin^2\left(\frac{\pi(k_2+2i-3)p}{q}\right) \ldots 4\sin^2\left(\frac{\pi(k_i+1)p}{q}\right). \tag{2.18}$$

We call $a_{p/q}(2i)$ the Kreft coefficients [15] because Kreft gave the expression eq. (2.18) when computing the determinant of the Harper's equation in the commensurate case. How to derive these coefficients is explained in Kreft's paper [15] (also see the Appendix A for details). Now $\Delta(zx, z/x, zy, z/y)$ rewrites as

$$\Delta(zx, z/x, zy, z/y) = b_{p/q}(z) - z^q(x^q + x^{-q} + y^q + y^{-q}). \tag{2.19}$$

Next, we focus on the numerator of $A(zx, z/x, zy, z/y, Q)$. Once the denominator is derived, the numerator becomes easier, because it just replaces the first column of $\Delta(zx, z/x, zy, z/y)$ by 1. More conveniently, we are only interested in its coefficient of $[x^0y^0]$. As it turns out

$$[x^0y^0] \begin{vmatrix} 1 & -z/x & 0 & \cdots & 0 & -zx \\ 1 & c_1 & -zx & \cdots & 0 & 0 \\ 1 & -z/x & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & c_{q-2} & -zx \\ 1 & 0 & 0 & \cdots & -z/x & c_{q-1} \end{vmatrix} = b_{p/q}(z) - \frac{z}{q} b'_{p/q}(z). \tag{2.20}$$

The specific detailed process of how to deal with the numerator and the denominator of $A(zx, z/x, zy, z/y, Q)$ is given in chapter 5 and appendix of Article 1.

To summarize, we get

$$[x^0y^0]A(zx, z/x, zy, z/y, Q) = [x^0y^0] \frac{b_{p/q}(z) - \frac{z}{q} b'_{p/q}(z)}{b_{p/q}(z) - z^q(x^q + x^{-q} + y^q + y^{-q})}.$$

Substitute the result above into eq. (2.14) and replace Q by $e^{2i\pi p/q}$, we get the generating function of $Z_n\left(e^{2i\pi p/q}\right)$

$$\sum_{n\geq 0} Z_n\left(e^{2i\pi p/q}\right) z^n = \left(1 - \frac{z b'_{p/q}(z)}{q b_{p/q}(z)}\right) \sum_{k\geq 0} \binom{2k}{k}^2 \left(\frac{z^q}{b_{p/q}(z)}\right)^{2k} \tag{2.21}$$

and it is equivalent to

$$\sum_{n\geq 0} Z_n\left(e^{2i\pi p/q}\right) z^n = \left(1 - \frac{z b'_{p/q}(z)}{q b_{p/q}(z)}\right) \frac{2}{\pi} K\left(\frac{16 z^{2q}}{b_{p/q}(z)^2}\right) \tag{2.22}$$

where K is the complete elliptic integral of the first kind:

$$K(x) = \int_0^1 \frac{1}{\sqrt{(1-t^2)(1-xt^2)}} dt,$$

see e.g. [[16], p. 161]. The explicit formula for the $Z_n(e^{2i\pi p/q})$'s (equivalently, the traces $\operatorname{Tr} H^n_{2\pi p/q}$) in terms of the Kreft coefficients $a_{p/q}(2i)$: for even $n > 0$,

$$Z_n\left(e^{2i\pi p/q}\right) = \operatorname{Tr} H^n_{2\pi p/q} = \frac{n}{q} \sum_{k\geq 0} \sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0 \\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor \ell_{\lfloor q/2\rfloor} = n/2-kq}} \frac{\binom{2k}{k}^2 \binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k} \prod_{j=1}^{\lfloor q/2\rfloor} a_{p/q}(2j)^{\ell_j} \tag{2.23}$$

See the appendix A.3 of Article 1 for the complete derivation of eq. (2.23).

2.4 Asymptotics

$n \to \infty$:

The generating function eq. (2.22) is useful for studying the asymptotic behavior when $n \to \infty$. The critical point here is in eq. (2.22) contains a complete elliptic integral of the first kind K, which has a logarithmic singularity at 1:

$$K(x) = -\frac{1}{2}\log(1-x) + O(1)$$

In eq. (2.22), they are at the points where $b_{p/q}(z) = \pm 4z^q$. So the asymptotic formulas can be obtained near these singularities. Please see the section 4 of Article 1 for more details.

$q \to \infty$:

From the definition eq. (2.4), when q goes to infinity, i.e. $Q \to 1$, the noncommutative random walks become commutative, the generating function for closed random walks with n total steps and m horizontal steps becomes

$$Z_{m,m,n/2-m,n/2-m}(1) = \binom{n}{m, m, n/2-m, n/2-m}$$

is the number of such closed paths. Then, $Z_n(e^{2i\pi p/q})$'s (equivalently, the traces $\mathrm{Tr}\, H^n_{2\pi p/q}$) for even $n > 0$, becomes

$$\lim_{q\to\infty} \mathrm{Tr} H^n_{2\pi p/q} = Z_n(1) = \sum_{m=0}^{n/2} Z_{m,m,n/2-m,n/2-m}(1) = \binom{n}{n/2}^2$$

This is the total number of closed paths with length n as mentioned before.

2.5 Summary and perspectives

In this chapter, thanks to the mapping between the algebraic area of lattice walks and the moments of Hofstadter Hamiltonian, by studying two-dimensional closed lattice walks, we have computed the generating function of $\mathrm{Tr}\, H^n_{2\pi p/q}$ in eq. (2.22). From this, one can derive the explicit formulas for these traces eq. (2.23) in terms of the Kreft coefficients given in eq. (2.18). We also studied the asymptotic behavior as $n \to \infty$. In Article 1, we show that it follows a law of the form $\mathrm{Tr}\, H^n_{2\pi p/q} \sim \frac{\beta}{n} \cdot \alpha^n$, where α and β are constants depending on p/q. Also, when $q \to \infty$, $\mathrm{Tr}\, H^n_{2\pi p/q} \sim \binom{n}{n/2}^2$, which is the total number of closed lattice walks with length n. More importantly, concerning random walks, a closed expression for the number $C_n(A)$ of closed random walks with length n enclosing a given algebraic area A remains an open issue. We made recent progress indicating that this information is encoded in the Kreft coefficients $a_{p/q}(2j)$ discussed above.

Article 1 : On the algebraic area of lattice walks and the Hofstadter model

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On the algebraic area of lattice walks and the Hofstadter model

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Abstract

We consider the generating function of the algebraic area of lattice walks, evaluated at a root of unity, and its relation to the Hofstadter model. In particular, we obtain an expression for the generating function of the nth moments of the Hofstadter Hamiltonian in terms of a complete elliptic integral, evaluated at a rational function. This, in turn, gives us both exact and asymptotic formulas for these moments.

Keywords: Hofstadter model, lattice walks, trace formula

1. Introduction

The algebraic area is the area enclosed by a curve, weighted by the winding number: if the curve moves around a region in a counterclockwise (positive) direction, its area counts as positive; otherwise it counts as negative. Moreover, if the curve winds around more than once, the area is counted with multiplicity. In this paper, we will be studying the algebraic area of two-dimensional lattice walks starting at the origin and moving up, down, left or right at each step. If the walk is not closed, we define its algebraic area as that of the closed walk obtained by connecting its endpoint with its starting point, adding on to the end of the walk the minimum necessary number of steps, first vertical, then horizontal (see figure 1).

Suppose that a lattice walk moves m_1 steps right, m_2 steps left, l_1 steps up and l_2 steps down. If, for example, $m_1 \geqslant m_2$ and $l_1 \geqslant l_2$, we add $l_1 - l_2$ steps down followed by $m_1 - m_2$ steps to the left in order to close the path. Let $C_{m_1,m_2,l_1,l_2}(A)$ be the number of such walks enclosing an algebraic area A. Finding the generating function for the $C_{m_1,m_2,l_1,l_2}(A)$'s, i.e.

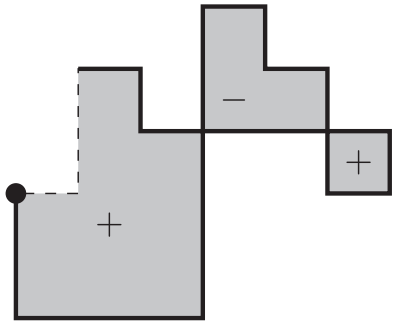

Figure 1. A lattice walk with algebraic area $9 - 3 + 1$.

$$Z_{m_1,m_2,l_1,l_2}(Q) = \sum_A C_{m_1,m_2,l_1,l_2}(A) Q^A, \tag{1}$$

is a difficult task, so far without a definite answer[3].

One can simplify by restricting this to closed lattice walks of a given length n (n is then necessarily even), i.e. walks with an equal number m of steps right/left and an equal number $n/2 - m$ of steps up/down, with $m \in \{0, 1, \ldots, n/2\}$, and by focusing on the generating function

$$Z_n(\mathrm{e}^{\mathrm{i}\gamma}) = \sum_{m=0}^{n/2} Z_{m,m,\frac{n}{2}-m,\frac{n}{2}-m}(\mathrm{e}^{\mathrm{i}\gamma}) \tag{2}$$

evaluated at $Q = \mathrm{e}^{\mathrm{i}\gamma}$, a root of unity. One reason for addressing this simpler question arises from the deep connection between the algebraic area distribution of random walks to the quantum mechanics of a charged particle in a perpendicular magnetic field. A paramount example is, in the continuous limit, Levy's law [3] for the algebraic area distribution of closed Brownian curves and its connection to the quantum Landau problem.

In the discrete case, the connection is to the quantum Hofstadter model [4] of a particle hopping on a two-dimensional lattice in a rational magnetic flux $\gamma = 2\pi p/q$, here counted in unit of the flux quantum. More precisely, $Z_n(\mathrm{e}^{\mathrm{i}\gamma})$ is mapped [5] to the nth moment of the Hofstadter Hamiltonian H_γ:

$$Z_n(\mathrm{e}^{\mathrm{i}\gamma}) = \mathrm{Tr}\, H_\gamma^n. \tag{3}$$

We will derive an expression for the multivariate generating function of Z_{m_1,m_2,l_1,l_2} as defined in (1), which even yields simple explicit formulas in some very special cases. The multivariate generating function is then specialized to the generating function of the $Z_n(\mathrm{e}^{\mathrm{i}\gamma})$s. This allows us to derive a closed expression for the $Z_n(\mathrm{e}^{\mathrm{i}\gamma})$s and thus, by virtue of (3), for the traces $\mathrm{Tr}\, H_\gamma^n$, in terms of the Kreft coefficients [6]. Not surprisingly, these coefficients encode, in a simple way, the quantum secular equation determining the Hofstadter spectrum. We will also use the generating function to study the asymptotic behaviour of $Z_n(\mathrm{e}^{\mathrm{i}\gamma})$ as $n \to \infty$ for fixed γ.

Needless to say that a better understanding of the moments of the Hofstadter Hamiltonian could, for example, allow for new interesting insights into the Hofstadter spectrum itself [7], in particular, in the irrational limit $p/q \to \alpha$ where both $p, q \to \infty$. These endeavours are left for future publications.

[3] For recent efforts in this direction see, for example, [1, 2].

2. Summary of results

Here is a brief outline of our results. As a first step, we will study the multivariate generating function

$$A(x_1, x_2, y_1, y_2, Q) = \sum_{m_1,m_2,l_1,l_2 \geqslant 0} Z_{m_1,m_2,l_1,l_2}(Q) x_1^{m_1} x_2^{m_2} y_1^{l_1} y_2^{l_2}$$

associated with $Z_{m_1,m_2,l_1,l_2}(Q)$. When Q is a qth root of unity, this function can be obtained from the solution of a linear system of equations: for certain auxiliary functions $A_1, A_2, \ldots, A_{q-1}$ and $A_0 = A(x_1, x_2, y_1, y_2, Q)$, we have

$$\begin{pmatrix} c_0 & -x_2 & 0 & \cdots & 0 & -x_1 \\ -x_1 & c_1 & -x_2 & \cdots & 0 & 0 \\ 0 & -x_1 & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} & -x_2 \\ -x_2 & 0 & 0 & \cdots & -x_1 & c_{q-1} \end{pmatrix} \cdot \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ \vdots \\ A_{q-2} \\ A_{q-1} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix},$$

where $c_k = 1 - Q^k y_1 - Q^{-k} y_2$; see the following section for details. Solving this system, we find that $A(x_1, x_2, y_1, y_2, Q)$ is a rational function, whose general form we investigate. For very small values of q, we even obtain explicit expressions for $Z_{m_1,m_2,l_1,l_2}(Q)$.

Specializing further, we concentrate on $Z_n(\mathrm{e}^{\mathrm{i}\gamma})$ as defined in (2), for $\gamma = 2\pi p/q$. We prove the generating function to be

$$\sum_{n \geqslant 0} Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q}) z^n = \left(1 - \frac{z b'_{p/q}(z)}{q b_{p/q}(z)}\right) \frac{2}{\pi} K\left(\frac{16 z^{2q}}{b_{p/q}(z)^2}\right), \tag{4}$$

where K is the complete elliptic integral of the first kind and the polynomial $b_{p/q}(z)$ is defined as

$$b_{p/q}(z) = 4z^q + \begin{vmatrix} 1-2z & -z & 0 & \cdots & 0 & -z \\ -z & 1 - 2z\cos\left(\frac{2\pi p}{q}\right) & -z & \cdots & 0 & 0 \\ 0 & -z & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & -z \\ -z & 0 & 0 & \cdots & -z & 1 - 2z\cos\left((q-1)\frac{2\pi p}{q}\right) \end{vmatrix}.$$

This is the main result of section 5, which also gives us an exact, albeit somewhat complicated, formula for $Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})$. Let $a(2), a(4), \ldots$ be, up to a change of sign, the coefficients of $b_{p/q}(z)$:

$$b_{p/q}(z) = -\sum_{i=0}^{\lfloor q/2 \rfloor} a_{p/q}(2i) z^{2i}.$$

For even $n > 0$, we have

$$Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q}) = \mathrm{Tr}\, H^n_{2\pi p/q} = \frac{n}{q} \sum_{k \geqslant 0} \sum_{\substack{\ell_1, \ell_2, \ldots, \ell_{\lfloor q/2 \rfloor} \geqslant 0 \\ \ell_1 + 2\ell_2 + \cdots + \lfloor q/2 \rfloor \ell_{\lfloor q/2 \rfloor} = n/2 - kq}} \times \frac{\binom{2k}{k}^2 \binom{\ell_1 + \ell_2 + \cdots + \ell_{\lfloor q/2 \rfloor} + 2k}{\ell_1, \ell_2, \ldots, \ell_{\lfloor q/2 \rfloor}, 2k}}{\ell_1 + \ell_2 + \cdots + \ell_{\lfloor q/2 \rfloor} + 2k} \prod_{j=1}^{\lfloor q/2 \rfloor} a(2j)^{\ell_j}.$$

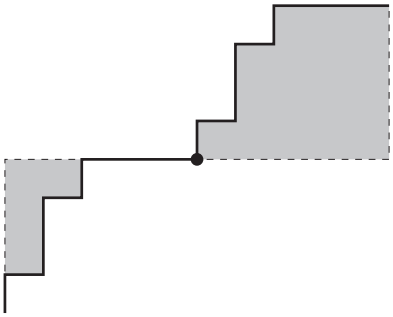

Figure 2. Illustration of (7).

From the explicit expression in (4), we can also deduce the analytic behaviour of the generating function which, in turn, yields the asymptotic behaviour of its coefficients. In section 6, we show that an asymptotic formula of the form

$$Z_n(e^{2\pi ip/q}) \sim \frac{\beta}{n} \cdot \alpha^n$$

holds for fixed p/q and even n as $n \to \infty$, where α and β are constants that depend on p/q.

3. The generating function for arbitrary walks

As mentioned before, we are interested in evaluating the generating function $Z_{m_1,m_2,l_1,l_2}(Q)$ when Q is a root of unity. Of course, we trivially have

$$Z_{m_1,m_2,l_1,l_2}(1) = \frac{(m_1 + m_2 + l_1 + l_2)!}{m_1!m_2!l_1!l_2!}.$$

Let us start with some symmetry properties: first of all, it is easy to see that

$$Z_{m_2,m_1,l_1,l_2}(Q) = Z_{m_1,m_2,l_2,l_1}(Q) = Z_{m_1,m_2,l_1,l_2}(Q^{-1}), \tag{5}$$

since reflections about the x- or y-axis only change the sign of the algebraic area. Moreover,

$$Z_{m_1,m_2,l_1,l_2}(Q) = Z_{l_1,l_2,m_1,m_2}(Q). \tag{6}$$

Finally, if we reverse the direction of a walk with m_1, m_2, l_1, l_2 steps right, left, up and down, respectively, the algebraic areas of the original and the reversed walk add up to $-(m_1 - m_2)(l_1 - l_2)$, which is particularly evident if the walk only moves in one quadrant, as in figure 2.

It follows that

$$Z_{m_2,m_1,l_2,l_1}(Q) = Q^{-(m_1-m_2)(l_1-l_2)} Z_{m_1,m_2,l_1,l_2}(Q^{-1}), \tag{7}$$

and combining this with (5) yields

$$Z_{m_1,m_2,l_1,l_2}(Q) = Q^{-(m_1-m_2)(l_1-l_2)} Z_{m_1,m_2,l_1,l_2}(Q^{-1}).$$

Thus,

$$Q^{(m_1-m_2)(l_1-l_2)/2} Z_{m_1,m_2,l_1,l_2}(Q)$$

is symmetric (in the sense that the coefficients of Q^k and Q^{-k} are equal for all k). If $|Q| = 1$ (in particular, if Q is a root of unity), this implies that

$$Q^{(m_1-m_2)(l_1-l_2)/2} Z_{m_1,m_2,l_1,l_2}(Q)$$

is real.

For further study, we define the multivariate generating function

$$A(x_1, x_2, y_1, y_2, Q) = \sum_{m_1,m_2,l_1,l_2 \geqslant 0} Z_{m_1,m_2,l_1,l_2}(Q) x_1^{m_1} x_2^{m_2} y_1^{l_1} y_2^{l_2}. \tag{8}$$

We distinguish the four possible cases for the last step: if the last step is vertical, then the algebraic area does not change. If it is a step to the left, the algebraic area changes exactly by the current y-coordinate; the same holds if the last step is a step to the right, but with opposite sign. It is now easy to see that the recursion

$$\begin{aligned} Z_{m_1,m_2,l_1,l_2}(Q) = {} & Z_{m_1,m_2,l_1-1,l_2}(Q) + Z_{m_1,m_2,l_1,l_2-1}(Q) \\ & + Q^{l_2-l_1} Z_{m_1-1,m_2,l_1,l_2}(Q) + Q^{l_1-l_2} Z_{m_1,m_2-1,l_1,l_2}(Q) \end{aligned}$$

holds, with initial values $Z_{0,0,0,0}(Q) = 1$ and $Z_{m_1,m_2,l_1,l_2}(Q) = 0$ whenever $\min(m_1, m_2, l_1, l_2) < 0$. We immediately obtain a functional equation for the multivariate generating function:

$$\begin{aligned} A(x_1, x_2, y_1, y_2, Q) = {} & 1 + y_1 A(x_1, x_2, y_1, y_2, Q) + y_2 A(x_1, x_2, y_1, y_2, Q) \\ & + x_1 A(x_1, x_2, Q^{-1} y_1, Q y_2, Q) + x_2 A(x_1, x_2, Q y_1, Q^{-1} y_2, Q). \end{aligned}$$

When Q is a root of unity, this turns into a finite system of linear equations. In the following, we will assume that Q is a (without loss of generality) primitive qth root of unity, so that $Q^q = 1$. Set

$$A_k = A(x_1, x_2, Q^k y_1, Q^{-k} y_2, Q),$$

which only depends on the residue class of k modulo q. Note that, in particular, $A_0 = A_q = A(x_1, x_2, y_1, y_2, Q)$. Now, we have

$$\begin{aligned} A_k &= A(x_1, x_2, Q^k y_1, Q^{-k} y_2, Q) \\ &= 1 + Q^k y_1 A(x_1, x_2, Q^k y_1, Q^{-k} y_2, Q) + Q^{-k} y_2 A(x_1, x_2, Q^k y_1, Q^{-k} y_2, Q) \\ &\quad + x_1 A(x_1, x_2, Q^{k-1} y_1, Q^{-k+1} y_2, Q) + x_2 A(x_1, x_2, Q^{k+1} y_1, Q^{-k-1} y_2, Q) \\ &= 1 + (Q^k y_1 + Q^{-k} y_2) A_k + x_1 A_{k-1} + x_2 A_{k+1}. \end{aligned}$$

The resulting linear system can be written in matrix form as

$$\begin{pmatrix} c_0 & -x_2 & 0 & \cdots & 0 & -x_1 \\ -x_1 & c_1 & -x_2 & \cdots & 0 & 0 \\ 0 & -x_1 & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} & -x_2 \\ -x_2 & 0 & 0 & \cdots & -x_1 & c_{q-1} \end{pmatrix} \cdot \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ \vdots \\ A_{q-2} \\ A_{q-1} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix},$$

where $c_k = 1 - Q^k y_1 - Q^{-k} y_2$. We can apply Cramer's rule to solve for A_0, which immediately shows that it is a rational function in x_1, x_2, y_1, y_2.

3.1. Special cases

For small values of q, the generating function is simple enough to extract explicit formulas for $Z_{m_1,m_2,l_1,l_2}(Q)$ from it.

- Specifically, we obtain for $q = 2$ (and thus $Q = -1$)

$$A_0 = A(x_1, x_2, y_1, y_2, -1) = \frac{1 + x_1 + x_2 + y_1 + y_2}{1 - (x_1 + x_2)^2 - (y_1 + y_2)^2}.$$

Expanding into a power series, we find

$$\begin{aligned} A(x_1, x_2, y_1, y_2, -1) &= \frac{1 + x_1 + x_2 + y_1 + y_2}{1 - (x_1 + x_2)^2 - (y_1 + y_2)^2} \\ &= (1 + x_1 + x_2 + y_1 + y_2) \sum_{n \geqslant 0} ((x_1 + x_2)^2 + (y_1 + y_2)^2)^n \\ &= (1 + x_1 + x_2 + y_1 + y_2) \sum_{n_1 \geqslant 0} \sum_{n_2 \geqslant 0} \binom{n_1 + n_2}{n_1} (x_1 + x_2)^{2n_1} (y_1 + y_2)^{2n_2} \\ &= \sum_{n_1 \geqslant 0} \sum_{n_2 \geqslant 0} \binom{n_1 + n_2}{n_1} ((x_1 + x_2)^{2n_1} (y_1 + y_2)^{2n_2} \\ &\quad + (x_1 + x_2)^{2n_1 + 1} (y_1 + y_2)^{2n_2} \\ &\quad + (x_1 + x_2)^{2n_1} (y_1 + y_2)^{2n_2 + 1}). \end{aligned}$$

From this expression, one reads off the coefficients easily:

$$Z_{m_1,m_2,l_1,l_2}(-1) = \begin{cases} \binom{\lfloor (m_1 + m_2 + l_1 + l_2)/2 \rfloor}{\lfloor (m_1 + m_2)/2 \rfloor} \binom{m_1 + m_2}{m_1} \binom{l_1 + l_2}{l_1} & \text{if } m_1 + m_2 \text{ or } l_1 + l_2 \text{ or both are even,} \\ 0 & \text{otherwise.} \end{cases}$$

- In general, however, the generating function A becomes more complicated. For $q = 3$, we immediately obtain

$$\frac{1 + x_1 + x_2 + y_1 + y_2 + x_1^2 + x_2^2 + y_1^2 + y_2^2 - x_1 x_2 - y_1 y_2 - Q x_1 y_1 - Q^{-1} x_1 y_2 - Q^{-1} x_2 y_1 - Q x_2 y_2}{1 - x_1^3 - x_2^3 - y_1^3 - y_2^3 - 3 x_1 x_2 - 3 y_1 y_2},$$

which gives us, for example, in the case where $m_1 - m_2 \equiv l_1 - l_2 \equiv 1 \bmod 3$,

$$Z_{m_1,m_2,l_1,l_2}(\mathrm{e}^{2\pi \mathrm{i}/3}) = -\mathrm{e}^{2\pi \mathrm{i}/3} \sum_{\substack{k=0 \\ k \equiv m_2 \bmod 3}}^{\min(m_1,m_2)} \sum_{\substack{j=0 \\ j \equiv l_2 \bmod 3}}^{\min(l_1,l_2)} 3^{k+j} \binom{\frac{m_1 + m_2 + l_1 + l_2 + k + j - 2}{3}}{k,\ j,\ \frac{m_1 - k - 1}{3},\ \frac{m_2 - k}{3},\ \frac{l_1 - j - 1}{3},\ \frac{l_2 - j}{3}}.$$

Similar formulas hold when $m_1 - m_2$ and $l_1 - l_2$ lie in other fixed residue classes modulo 3.

- An elegant formula is obtained for $Q = \pm i$ (i.e. $q = 4$) if we count walks by the total number of horizontal and vertical steps: we have

$$\sum_{m_1 + m_2 = m} \sum_{l_1 + l_2 = l} Z_{m_1,m_2,l_1,l_2}(\pm i) = 2^{m+l} \binom{\lfloor m/2 \rfloor + \lfloor l/2 \rfloor}{\lfloor m/2 \rfloor},$$

which is obtained from the generating function

$$A(x, x, y, y, \pm i) = \frac{1 + 2x + 2y + 4xy}{1 - 4x^2 - 4y^2}.$$

Note that we also have

$$\sum_{m_1+m_2=m}\sum_{l_1+l_2=l} Z_{m_1,m_2,l_1,l_2}(-1) = 2^{m+l}\begin{pmatrix} \lfloor m/2\rfloor + \lfloor l/2\rfloor \\ \lfloor m/2\rfloor \end{pmatrix},$$

except when m, l are both odd, in which case the sum evaluates to 0.

3.2. The general shape

We know now that A is a rational function if evaluated at a root of unity Q. Let us show that it always has the following shape:

$$A(x_1, x_2, y_1, y_2, Q) = \frac{U(x_1, x_2, y_1, y_2)}{1 - x_1^q - x_2^q - y_1^q - y_2^q \;+\; V(x_1x_2, y_1y_2)}, \tag{9}$$

where U, V are polynomials and V is symmetric (in its two variables) and has only real coefficients (and constant coefficient 0). By Cramer's rule, we have

$$A(x_1, x_2, y_1, y_2, Q) = \frac{\begin{vmatrix} 1 & -x_2 & 0 & \cdots & 0 & -x_1 \\ 1 & c_1 & -x_2 & \cdots & 0 & 0 \\ 1 & -x_1 & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & c_{q-2} & -x_2 \\ 1 & 0 & 0 & \cdots & -x_1 & c_{q-1} \end{vmatrix}}{\begin{vmatrix} c_0 & -x_2 & 0 & \cdots & 0 & -x_1 \\ -x_1 & c_1 & -x_2 & \cdots & 0 & 0 \\ 0 & -x_1 & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} & -x_2 \\ -x_2 & 0 & 0 & \cdots & -x_1 & c_{q-1} \end{vmatrix}}, \tag{10}$$

where $c_k = 1 - Q^k y_1 - Q^{-k} y_2$ as before. Let us show that the determinant Δ which appears in the denominator of (10) is indeed of the form $1 - x_1^q - x_2^q - y_1^q - y_2^q + V(x_1x_2, y_1y_2)$, where V is symmetric and has real coefficients. This is done in the following steps:

- We note that the determinant Δ is a polynomial in x_1, x_2, y_1, y_2 with total degree q.
- If we replace y_1 by Qy_1 and y_2 by $Q^{-1}y_2$, we end up with the determinant

$$\begin{vmatrix} c_1 & -x_2 & 0 & \cdots & 0 & -x_1 \\ -x_1 & c_2 & -x_2 & \cdots & 0 & 0 \\ 0 & -x_1 & c_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-1} & -x_2 \\ -x_2 & 0 & 0 & \cdots & -x_1 & c_0 \end{vmatrix},$$

  which is also obtained from the original determinant Δ by moving the first row and column to the end; hence, the value does not change. This means that the only nonzero terms in Δ (seen as a polynomial in y_1 and y_2 only) that can have a nonzero coefficient are y_1^q, y_2^q and all powers of y_1y_2.
- By expansion with respect to the last row and the last column, we obtain

$$\begin{vmatrix} c_0 & -x_2 & 0 & \cdots & 0 & -x_1 \\ -x_1 & c_1 & -x_2 & \cdots & 0 & 0 \\ 0 & -x_1 & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} & -x_2 \\ -x_2 & 0 & 0 & \cdots & -x_1 & c_{q-1} \end{vmatrix}$$

$$= -x_1{}^q - x_2^q + c_{q-1} \begin{vmatrix} c_0 & -x_2 & 0 & \cdots & 0 \\ -x_1 & c_1 & -x_2 & \cdots & 0 \\ 0 & -x_1 & c_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} \end{vmatrix}$$

$$-x_1x_2 \begin{vmatrix} c_0 & -x_2 & 0 & \cdots & 0 \\ -x_1 & c_1 & -x_2 & \cdots & 0 \\ 0 & -x_1 & c_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-3} \end{vmatrix} - x_1x_2 \begin{vmatrix} c_1 & -x_2 & \cdots & 0 & 0 \\ -x_1 & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{q-3} & -x_2 \\ 0 & 0 & \cdots & -x_1 & c_{q-2} \end{vmatrix}.$$

It is easy to see that the determinants

$$D_k = \begin{vmatrix} u_1 & -x_2 & \cdots & 0 & 0 \\ -x_1 & u_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & u_{k-1} & -x_2 \\ 0 & 0 & \cdots & -x_1 & u_k \end{vmatrix}, \tag{11}$$

where the u_j are arbitrary coefficients, satisfy the recursion $D_k = u_kD_{k-1} - x_1x_2D_{k-2}$ and are, therefore, polynomials in x_1x_2.

- Combining the observations in the last two items, we see that the determinant is of the form

$$\Delta(x_1, x_2, y_1, y_2) = -x_1^q - x_2^q - y_1^q - y_2^q + R(x_1x_2, y_1y_2)$$

for some polynomial R. If we set $x_1 = x_2 = y_1 = y_2 = 0$, the determinant evaluates to 1, so we can write $R(x_1x_2, y_1y_2) = 1 + V(x_1x_2, y_1y_2)$, where the constant coefficient of V is zero. It remains to show that V is symmetric and has only real coefficients.

If we exchange y_1 and y_2, then $\Delta(x_1, x_2, y_1, y_2) = 1 - x_1^q - x_2^q - y_1^q - y_2^q + V(x_1x_2, y_1y_2)$ obviously does not change. On the other hand, $c_j = 1 - Q^jy_1 - Q^{-j}y_2$ becomes $1 - Q^jy_2 - Q^{-j}y_1 = \overline{c_j}$. All other matrix entries are real and, therefore, equal to their conjugates (if we consider x_1, x_2, y_1, y_2 as real variables for the moment). This means that Δ is equal to its own conjugate, so it has only real coefficients.

- Finally, we observe that Δ is an irreducible polynomial: suppose for contradiction that it can be factorized into two nonconstant factors. If we set $x_2 = y_2 = 0$, we obtain a factorization of $1 - x_1^q - y_1^q$, which is irreducible: its factorization as a polynomial in x_1 is

$$1 - x_1^q - y_1^q = -\prod_{j=0}^{q-1} (x_1 - Q^j(1 - y_1^q)^{1/q}),$$

and since $1 - y_1^q$ is not a power of a polynomial, there is no factorization of $1 - x_1^q - y_1^q$ into polynomials.

Thus, the factorization of Δ becomes $(1 - x_1^q - y_1^q) \cdot 1$ for $x_2 = y_2 = 0$. So the first factor has a total degree (at least) q, which is already the total degree of Δ. This means that the second factor has to be constant, and we reach a contradiction.

Therefore,

$$A(x_1, x_2, y_1, y_2, Q) = \frac{U(x_1, x_2, y_1, y_2)}{1 - x_1^q - x_2^q - y_1^q - y_2^q + V(x_1 x_2, y_1 y_2)}$$

is in its lowest terms. In view of symmetry condition (6), the function does not change when x_1, x_2 are replaced by y_1, y_2 respectively. Thus, V must be symmetric.

4. Hofstadter quantum mechanics

As stated in the introduction, $Z_{m_1,m_2,l_1,l_2}(Q)$ happens to be of interest for the quantum Hofstadter model [4], thanks to the mapping (3) between the algebraic area generating function for closed walks of length n evaluated at $Q = \mathrm{e}^{\mathrm{i}\gamma}$ and the nth moment of the quantum Hofstadter Hamiltonian $\mathrm{Tr}\, H_\gamma^n$. Of particular interest is the commensurate flux $\gamma = 2\pi p/q$, where p and q are relatively prime, so that Q is a primitive qth root of unity.

In the Landau gauge, the Hofstadter Hamiltonian is

$$H_\gamma = T_x + T_x^{-1} + T_y + T_y^{-1},$$

where the lattice hopping operators T_x and T_y obey the commutation relation

$$T_x T_y = \mathrm{e}^{-\mathrm{i}\gamma} T_y T_x.$$

They act on a state $\Psi_{m,n}$ at lattice site $\{m, n\}$ as follows:

$$T_x \Psi_{m,n} = \Psi_{m+1,n}, \quad T_y \Psi_{m,n} = \mathrm{e}^{\mathrm{i}\gamma m} \Psi_{m,n+1}.$$

Using translation invariance in the y direction one sets $\Psi_{m,n} = \mathrm{e}^{\mathrm{i}nk_y} \Phi_m$ to get the eigenenergy Harper equation

$$\Phi_{m+1} + \Phi_{m-1} + 2\cos(k_y + \gamma m)\Phi_m = E\Phi_m.$$

In the commensurate case $\gamma = 2\pi p/q$ one has on the horizontal axis a periodic model with period q, so $\Phi_{m+q} = \mathrm{e}^{\mathrm{i}qk_x} \Phi_m$. All this amounts to the $q \times q$ matrix $m_{p/q}(E, k_x, k_y)$ acting with zero output on the q-components eigenvector $\{\Phi_0, \Phi_1, \ldots, \Phi_{q-1}\}$:

$$\begin{pmatrix} 2\cos(k_y) - E & 1 & 0 & \cdots & 0 & \mathrm{e}^{-\mathrm{i}qk_x} \\ 1 & 2\cos\left(k_y + \frac{2\pi p}{q}\right) - E & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ \mathrm{e}^{\mathrm{i}qk_x} & 0 & 0 & \cdots & 1 & 2\cos\left(k_y + (q-1)\frac{2\pi p}{q}\right) - E \end{pmatrix}$$

$$\cdot \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{q-2} \\ \Phi_{q-1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}. \tag{12}$$

The q eigenenergies $E_r(k_x, k_y)$ with $r = 1, \ldots, q$ are solutions of the secular equation

$$\det(m_{p/q}(E, k_x, k_y)) = 0,$$

which, thanks to the identity

$$\det(m_{p/q}(E, k_x, k_y)) = \det(m_{p/q}(E, 0, 0)) - 2(-1)^q(\cos(qk_x) - 1 + \cos(qk_y) - 1),$$

can be rewritten [8] as

$$\det(m_{p/q}(E, 0, 0)) = 2(-1)^q(\cos(qk_x) - 1 + \cos(qk_y) - 1). \tag{13}$$

The trace is defined as

$$\mathrm{Tr}\, H^n_{2\pi p/q} = \frac{1}{q}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}k_x}{2\pi}\frac{\mathrm{d}k_y}{2\pi}\sum_{r=1}^{q} E_r^n(k_x, k_y), \tag{14}$$

where one sums over the q eigenenergies $E_r(k_x, k_y)$ of the Hofstadter Hamiltonian at power n and integrates over the quasimomenta $k_x \in [-\pi, \pi]$ and $k_y \in [-\pi, \pi]$. So in (14), computing[4] $\mathrm{Tr}\, H^n_{2\pi p/q}$ amounts to:

- first evaluating the determinant of $m_{p/q}(E, 0, 0)$, a polynomial of degree q in E;
- next solving the secular equation (13) for the q eigenenergies $E_r(k_x, k_y)$; it can be done numerically and leads to the Hofstadter butterfly when the eigenenergies are plotted against p/q;
- finally summing and integrating to get the trace of the Hofstadter Hamiltonian at a power n.

Evaluating $\mathrm{Tr}\, H^n_{2\pi p/q}$ in this way (i.e. from its definition (14) in terms of the quantum eigenenergies) is clearly a difficult task. We are going to address this question not from the quantum Hofstadter side, but rather via the mapping (3) from the lattice walks combinatorial side, by evaluating $Z_n(Q) = \sum_{m=0}^{n/2} Z_{m,m,\frac{n}{2}-m,\frac{n}{2}-m}(Q)$ at $Q = \mathrm{e}^{2\mathrm{i}\pi p/q}$.

[4] For earlier attempts to compute such traces, see, for example [9].

5. The trace formula

In the following, we will derive an expression for the generating function $\sum_{n\geqslant 0} Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})z^n$ in terms of a complete elliptic integral, evaluated at a rational function. To this end, we first specialize the multivariate generating function (8) from the previous section, i.e.

$$A(x_1, x_2, y_1, y_2, Q) = \sum_{m_1,m_2,l_1,l_2\geqslant 0} Z_{m_1,m_2,l_1,l_2}(Q) x_1^{m_1} x_2^{m_2} y_1^{l_1} y_2^{l_2}.$$

One observes that $\sum_{m=0}^{n/2} Z_{m,m,\frac{n}{2}-m,\frac{n}{2}-m}(Q)$ can be obtained directly from $A(x_1, x_2, y_1, y_2, Q)$ by setting $x_1 \to zx$, $x_2 \to z/x$, $y_1 \to zy$ and $y_2 \to z/y$ and looking at the coefficient where the exponents of x and y are 0 (enforcing $m_1 - m_2 = 0$ and $l_1 - l_2 = 0$) and the exponent of z is n (which corresponds to the condition $m_1 + m_2 + l_1 + l_2 = n$).

Let us now look for the coefficient of x^0y^0 in $A(zx, z/x, zy, z/y, Q)$ evaluated at Q, a root of unity: we already know from (9) that the determinant Δ in the denominator has the form $\Delta(x_1, x_2, y_1, y_2) = 1 - x_1^q - x_2^q - y_1^q - y_2^q + V(x_1x_2, y_1y_2)$, so it simplifies to

$$\Delta(zx, z/x, zy, z/y) = 1 - z^q(x^q + x^{-q} + y^q + y^{-q}) + V(z^2, z^2).$$

For $x = y = 1$, we get $\Delta(z, z, z, z) = 1 - 4z^q + V(z^2, z^2)$, which is the determinant of the $q \times q$ matrix

$$\begin{pmatrix} 1-2z & -z & 0 & \cdots & 0 & -z \\ -z & 1-2z\cos\left(\frac{2\pi p}{q}\right) & -z & \cdots & 0 & 0 \\ 0 & -z & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & -z \\ -z & 0 & 0 & \cdots & -z & 1-2z\cos\left((q-1)\frac{2\pi p}{q}\right) \end{pmatrix}. \tag{15}$$

Hence, we define

$$b_{p/q}(z) = \Delta(z, z, z, z) + 4z^q = 1 + V(z^2, z^2),$$

a polynomial of degree $2\lfloor q/2\rfloor$, with coefficients $-a_{p/q}(2i)$:

$$b_{p/q}(z) = -\sum_{i=0}^{\lfloor q/2\rfloor} a_{p/q}(2i) z^{2i}. \tag{16}$$

Now, $\Delta(zx, z/x, zy, z/y)$ rewrites as

$$\Delta(zx, z/x, zy, z/y) = b_{p/q}(z) - z^q(x^q + x^{-q} + y^q + y^{-q}). \tag{17}$$

Next, we focus on the numerator of $A(zx, z/x, zy, z/y, Q)$. It follows from (17) that the expansion of $1/\Delta$ only contains powers of x and y whose exponents are multiples of $-q$ and q. On the other hand, in view of its definition as a determinant in (10), the numerator only contains powers of x and y with exponents between $-(q-1)$ and $q-1$. Since we are only interested in the coefficient of x^0y^0, we can focus on this coefficient in the numerator as well, as the other terms will only give rise to monomials in the expansion of $A(zx, z/x, zy, z/y, Q)$ where the exponents of x and y are not simultaneously multiples of q.

As it turns out, the coefficient of x^0y^0 in the numerator can also be expressed in terms of the polynomial $b_{p/q}$:

$$[x^0y^0]\begin{vmatrix} 1 & -z/x & 0 & \cdots & 0 & -zx \\ 1 & c_1 & -z/x & \cdots & 0 & 0 \\ 1 & -zx & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & c_{q-2} & -z/x \\ 1 & 0 & 0 & \cdots & -zx & c_{q-1} \end{vmatrix} = b_{p/q}(z) - \frac{z}{q}b'_{p/q}(z). \tag{18}$$

A proof of this identity is given in the appendix.

Putting everything together that has been established so far for the denominator and numerator of $A(zx, z/x, zy, z/y, Q)$, we are left with

$$[x^0y^0]A(zx, z/x, zy, z/y, Q) = [x^0y^0]\frac{b_{p/q}(z) - \frac{z}{q}b'_{p/q}(z)}{b_{p/q}(z) - z^q(x^q + x^{-q} + y^q + y^{-q})}.$$

This can be expanded as

$$\begin{aligned}\frac{b_{p/q}(z) - \frac{z}{q}b'_{p/q}(z)}{b_{p/q}(z) - z^q(x^q + x^{-q} + y^q + y^{-q})} &= \left(1 - \frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\right) \\ &\times \frac{1}{1 - \frac{z^q}{b_{p/q}(z)}(x^q + x^{-q} + y^q + y^{-q})} \\ &= \left(1 - \frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\right)\sum_{k\geqslant 0}\left(\frac{z^q}{b_{p/q}(z)}\right)^k (x^q + x^{-q} + y^q + y^{-q})^k.\end{aligned}$$

The coefficient of x^0y^0 in $(x^q + x^{-q} + y^q + y^{-q})^k$ is $\binom{k}{k/2}^2$ if k is even and 0 otherwise, so that this procedure finally coalesces to

$$\sum_{n\geqslant 0} Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})z^n = \left(1 - \frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\right)\sum_{k\geqslant 0}\binom{2k}{k}^2\left(\frac{z^q}{b_{p/q}(z)}\right)^{2k}. \tag{19}$$

The series $\sum_{k\geqslant 0}\binom{2k}{k}^2 x^k$ can be expressed as $\frac{2}{\pi}K(16x)$, where K is the complete elliptic integral of the first kind:

$$K(x) = \int_0^1 \frac{1}{\sqrt{(1 - t^2)(1 - xt^2)}}\,\mathrm{d}t,$$

see, for example, [10, p 161]. To conclude, we have

$$\sum_{n\geqslant 0} Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})z^n = \left(1 - \frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\right)\frac{2}{\pi}K\left(\frac{16z^{2q}}{b_{p/q}(z)^2}\right). \tag{20}$$

For example, when $p = 1$, $q = 8$, i.e. $Q = \exp(2\pi i/8)$, we get

$$b_{1/8}(z) = 1 - 16z^2 + (72 - 8\sqrt{2})z^4 - (96 - 32\sqrt{2})z^6 + 4z^8$$

and

$$\begin{aligned}\sum_{n\geqslant 0} Z_n(\mathrm{e}^{2\pi\mathrm{i}/8})z^n = 1 &+ 4z^2 + (28 + 4\sqrt{2})z^4 + (232 + 72\sqrt{2})z^6 \\ &+ (2140 + 960\sqrt{2})z^8 + \cdots.\end{aligned}$$

Finding the generating function (20) for the $Z_n(e^{2i\pi p/q})$s, or equivalently for the traces $\mathrm{Tr}\, H^n_{2\pi p/q}$, narrows it down to determining the polynomial $b_{p/q}(z)$, i.e. the coefficients $a_{p/q}(2i)$ as defined in (16). But these coefficients of $b_{p/q}(z)$ in the expansion of the determinant of the matrix (15) are in one-to-one correspondence with those of the expansion of the determinant of the Hofstadter matrix $m_{p/q}(E, 0, 0)$ in (12), which is a consequence of the identity[5]

$$(-1)^q E^q b_{p/q}(1/E) = \det(m_{p/q}(E, 0, 0)) + 4(-1)^q. \tag{21}$$

So the Hofstadter secular energy equation (13) becomes

$$E^q b_{p/q}(1/E) = 2(\cos(qk_x) + \cos(qk_y)).$$

In view of (21), the $a_{p/q}(2i)$s can be identified with the Kreft coefficients $\mathrm{c}_{p/q}(2i)$ defined in [6]:

$$\det(m_{p/q}(E, 0, 0)) + 4(-1)^q = \sum_{i=\frac{q}{2}-\left[\frac{q}{2}\right]}^{q} \mathrm{c}_{p/q}(2i)E^{2i},$$

i.e.

$$a_{p/q}(2i) = \mathrm{c}_{p/q}(q - 2i)(-1)^{q+1},$$

and one ends up with

$$\begin{aligned} a_{p/q}(2i) = (-1)^{i+1} \sum_{k_1=0}^{q-2i} \sum_{k_2=0}^{k_1} \cdots \sum_{k_i=0}^{k_{i-1}} & 4\sin^2\left(\frac{\pi(k_1 + 2i - 1)p}{q}\right) \\ & \times 4\sin^2\left(\frac{\pi(k_2 + 2i - 3)p}{q}\right) \cdots 4\sin^2\left(\frac{\pi(k_i + 1)p}{q}\right) \end{aligned} \tag{22}$$

(see the appendix for some remarks on these coefficients).

[5] To see why (21) holds, recall that by definition, $b_{p/q}(z) = \Delta(z, z, z, z) + 4z^q$, where $\Delta(z, z, z, z)$ is the determinant of the matrix in (15). It follows that

$$(-1)^q E^q b_{p/q}(1/E) = (-1)^q E^q \Delta(1/E, 1/E, 1/E, 1/E) + 4(-1)^q,$$

and

$$\begin{aligned} &(-1)^q E^q \Delta(1/E, 1/E, 1/E, 1/E) \\ &= (-E)^q \begin{vmatrix} 1 - 2/E & -1/E & 0 & \cdots & 0 & -1/E \\ -1/E & 1 - 2\cos\left(\frac{2\pi p}{q}\right)/E & -1/E & \cdots & 0 & 0 \\ 0 & -1/E & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & -1/E \\ -1/E & 0 & 0 & \cdots & -1/E & 1 - 2\cos\left((q-1)\frac{2\pi p}{q}\right)/E \end{vmatrix} \\ &= \begin{vmatrix} 2 - E & 1 & 0 & \cdots & 0 & 1 \\ 1 & 2\cos\left(\frac{2\pi p}{q}\right) - E & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ 1 & 0 & 0 & \cdots & 1 & 2\cos\left((q-1)\frac{2\pi p}{q}\right) - E \end{vmatrix} \end{aligned}$$

is the determinant of $m_{p/q}(E, 0, 0)$.

The elliptic integral K satisfies a second-order differential equation with polynomial coefficients; therefore, so does the generating function $\sum_{n\geqslant 0} Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})z^n$ (although it is generally a rather complicated differential equation), i.e. it is holonomic. For example, when $q=4$, (i.e. $Q=i$), we have

$$\begin{aligned}
&(4096z^{15}-14848z^{13}+17920z^{11}-9696z^9+2720z^7-412z^5+32z^3-z)\\
&\times\left(\sum_{n\geqslant 0}Z_n(i)z^n\right)''\\
&+(20480z^{14}-54784z^{12}+52480z^{10}-26464z^8+7040z^6-940z^4+56z^2-1)\\
&\times\left(\sum_{n\geqslant 0}Z_n(i)z^n\right)'\\
&+(16384z^{13}-32768z^{11}+23040z^9-7168z^7+2112z^5-320z^3+16z)\\
&\times\left(\sum_{n\geqslant 0}Z_n(i)z^n\right)=0.
\end{aligned}$$

This means that its coefficients, i.e. the traces $\mathrm{Tr}\,H^n_{2\pi p/q}$, satisfy a linear recursion with polynomial coefficients. For example, when $q=4$, the linear recursion is

$$\begin{aligned}
n^2Z_n(i)=&(4096n^2-98304n+589824)Z_{n-14}(i)\\
&+(-14848n^2+316416n-1691648)Z_{n-12}(i)\\
&+(17920n^2-323840n+1469440)Z_{n-10}(i)\\
&+(-9696n^2+138368n-493568)Z_{n-8}(i)\\
&+(2720n^2-28320n+74112)Z_{n-6}(i)\\
&+(-412n^2+2768n-4800)Z_{n-4}(i)\\
&+(32n^2-104n+96)Z_{n-2}(i).
\end{aligned}\tag{23}$$

It is also possible to give an explicit sum formula for the $Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})$'s (equivalently, the traces $\mathrm{Tr}\,H^n_{2\pi p/q}$) in terms of the Kreft coefficients $a(2i)$: for even $n>0$:

$$\begin{aligned}
Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})=\mathrm{Tr}\,H^n_{2\pi p/q}=&\frac{n}{q}\sum_{k\geqslant 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geqslant 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-kq}}\\
&\times\frac{\binom{2k}{k}^2\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}\prod_{j=1}^{\lfloor q/2\rfloor}a_{p/q}(2j)^{\ell_j},
\end{aligned}\tag{24}$$

see the appendix for a complete derivation. For small values of q, this simplifies quite considerably (see [9]): for $q=2$, we have

$$Z_n(-1)=\sum_{0\leqslant k\leqslant n/4}\binom{2k}{k}^2\binom{n/2}{2k}2^{n-4k}.$$

Likewise, we get the following formula for $q=3$:

$$Z_n(\mathrm{e}^{\pm 2\pi\mathrm{i}/3})=\frac{2n}{3}\sum_{0\leqslant k\leqslant n/6}\binom{2k}{k}^2\binom{n/2-k}{2k}\frac{6^{n/2-3k}}{n-2k}.$$

For a given n, when q increases as well as p—having in mind the irrational limit where both p and $q \to \infty$—the number of summation indices in (24) increases as $\lfloor q/2 \rfloor + 1$. Clearly the physical results for, say, $p/q = 1/2$ and $p/q = 0.5000001$ should be very close to each other, at least if n is not too large (for very large n, the difference actually goes to infinity). And yet, the first generating function is a two-dimensional sum while the second is a 5 000 001-dimensional sum. This situation is reminiscent of, for example, the density correlation of the Calogero model obtained in [11] where multi-dimensional integrals of greatly varying size are obtained for close rational Calogero couplings.

As a final remark, we note that the generating function in (20) is identical to

$$\int_{-4}^{4} \rho_{p/q}(E) \frac{1}{1 - zE} \mathrm{d}E = \left(1 - \frac{z b'_{p/q}(z)}{q b_{p/q}(z)}\right) \frac{2}{\pi} K\left(\frac{16 z^{2q}}{b_{p/q}(z)^2}\right), \tag{25}$$

where $\rho_{p/q}(E)$ is the Hofstadter density of states:

$$\rho_{p/q}(E) = \frac{1}{2\pi^2 q} |(E^q b_{p/q}(1/E))'| K\left(1 - \left(\frac{E^q b_{p/q}(1/E)}{4}\right)^2\right)$$

when $\left| \frac{E^q b_{p/q}(1/E)}{4} \right| < 1$, and zero otherwise [12]. One can show that (25) is directly related to the known identity

$$\int_{-4}^{4} K\left(1 - \frac{s^2}{16}\right) \frac{1}{1 - zs} \, \mathrm{d}s = 4\pi K(16 z^2) \tag{26}$$

for the elliptic integral K.

6. Asymptotics

From the representation (20) of the generating function, namely

$$F_{p/q}(z) = \sum_{n \geqslant 0} Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q}) z^n = \left(1 - \frac{z b'_{p/q}(z)}{q b_{p/q}(z)}\right) \frac{2}{\pi} K\left(\frac{16 z^{2q}}{b_{p/q}(z)^2}\right),$$

the asymptotic behaviour of $Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})$ as $n \to \infty$ for fixed p/q can be obtained by standard means. We note that the elliptic integral K has a logarithmic singularity at 1:

$$K(x) = -\frac{1}{2} \log(1 - x) + O(1)$$

as $x \to 1$. This logarithmic singularity carries over to singularities of $F_{p/q}(z)$ at the points where $b_{p/q}(z) = \pm 4 z^q$. For example, if $p/q = 1/2$, we have $b_{1/2}(z) = 1 - 4z^2$, which gives us singularities at $z = \pm 1/\sqrt{8}$. At these singularities, the asymptotic behaviour of $F_{1/2}(z)$ is given by

$$F_{1/2}(z) = -\frac{2}{\pi} \log(1 - \sqrt{8}\, z) + O(1)$$

and

$$F_{1/2}(z) = -\frac{2}{\pi} \log(1 + \sqrt{8}\, z) + O(1),$$

respectively. Application of Flajolet-Odlyzko singularity analysis [13] directly yields

$$Z_n(-1) = [z^n]F_{1/2}(z)\begin{cases}\sim\frac{4}{\pi n}\cdot 8^{n/2} & n \text{ even},\\ =0 & n \text{ odd}.\end{cases}$$

Similarly, for $p/q = 1/3$, we have $b_{1/3}(z) = 1 - 6z^2$; the dominant singularities (those closest to the origin) of $F_{1/3}(z)$ are $z = \pm\frac{\sqrt{3}-1}{2}$. We have

$$F_{1/3}(z) = -\frac{2+\sqrt{3}}{\pi}\log\left(1 - \frac{2z}{\sqrt{3}-1}\right) + O(1)$$

as $z \to \frac{\sqrt{3}-1}{2}$ and an analogous asymptotic formula as $z \to -\frac{\sqrt{3}-1}{2}$. Singularity analysis gives us

$$Z_n(\mathrm{e}^{2\pi\mathrm{i}/3}) = [z^n]F_{1/3}(z)\begin{cases}\sim\frac{4+2\sqrt{3}}{\pi n}\cdot(1+\sqrt{3})^n & n \text{ even},\\ =0 & n \text{ odd}.\end{cases}$$

In the same way, one obtains an asymptotic formula of the form

$$Z_n(\mathrm{e}^{2\pi\mathrm{i}p/q}) = [z^n]F_{p/q}(z) \sim \frac{\beta}{n}\cdot\alpha^n$$

for arbitrary fixed p/q and even n as $n \to \infty$, where α and β depend on p/q. The table lists a few further values:

$\frac{p}{q}$	$\frac{1}{4}$ or $\frac{3}{4}$	$\frac{1}{5}$ or $\frac{4}{5}$	$\frac{2}{5}$ or $\frac{3}{5}$	$\frac{1}{6}$ or $\frac{5}{6}$
α	$\sqrt{8}$	$\frac{1+\sqrt{5}+\sqrt{70+2\sqrt{5}}}{4}$	$\frac{3+\sqrt{5}}{2}$	$\sqrt{5+\sqrt{21}}$
β	$\frac{16}{\pi}$	$\frac{19+11\sqrt{5}+\sqrt{670+298\sqrt{5}}}{2\pi}$	$\frac{7+3\sqrt{5}}{\pi}$	$\frac{56+12\sqrt{21}}{\pi}$

7. Conclusion

Making use of the connection to the algebraic area of lattice walks, we are able to compute the generating function of the traces $\mathrm{Tr}\, H^n_{2\pi p/q}$ of the Hofstadter Hamiltonian for any fixed rational number p/q—see (20). From this, one can derive both recursive (see (23)) and explicit formulas (see (24)) for these traces. The building blocks of (24) are the Kreft coefficients in (22) (see also section 6.2 in the appendix). When q is small, these formulas turn out to be quite simple. The generating function can also be used to study the asymptotic behaviour as $n \to \infty$, which follows a law of the form $\mathrm{Tr}\, H_{2\pi p/q} \sim \frac{\beta}{n}\cdot\alpha^n$, where α and β are constants depending on p/q.

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Appendix

A.1. Proof of (18)

(1) Consider the bivariate determinant

$$B(y,z)=\begin{vmatrix} c_0 & -z & 0 & \cdots & 0 & -z \\ -z & c_1 & -z & \cdots & 0 & 0 \\ 0 & -z & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} & -z \\ -z & 0 & 0 & \cdots & -z & c_{q-1} \end{vmatrix},$$

with $c_k = 1 - z(Q^k y - Q^{-k} y^{-1})$. It is *a priori* clear that the determinant $B(y, z)$ can only contain the powers $y^{-q}, y^{-q+1}, \ldots, y^{-1}, y^0, y^1, \ldots, y^{q-1}, y^q$ and $z^0, z^1, \ldots, z^q$, respectively. If y is replaced by Qy, then c_k becomes c_{k+1} (and c_{q-1} becomes c_0), so this amounts to a cyclic permutation of the diagonal entries. Since this does not change the value of the determinant, we have $B(Qy, z) = B(y, z)$. The only powers of y that stay invariant under the transformation $y \mapsto Qy$ are y^{-q}, y^0 and y^q, so these are the only powers that actually occur in $B(y, z)$. Moreover, making use of the fact that y and y^{-1} only occur in the diagonal entries, one easily finds that

$$[y^q]B(y,z) = [y^q]\prod_{k=0}^{q-1} c_k = (-1)^q Q^{q(q-1)/2} z^q = \pm z^q,$$

and likewise $[y^{-q}]B(y, z) = \pm z^q$. Since the term involving z^q cancels in $B(y, z) - \frac{z}{q}\frac{\partial}{\partial z}B(y, z)$, this means that $B(y, z) - \frac{z}{q}\frac{\partial}{\partial z}B(y, z)$ does not contain y at all (i.e. it is independent of y). Thus, we can also write

$$\begin{aligned} b_{p/q}(z) - \frac{z}{q} b'_{p/q}(z) &= B(1,z) - \frac{z}{q}\frac{\partial}{\partial z}B(1,z) \\ &= [y^0]\left(B(y,z) - \frac{z}{q}\frac{\partial}{\partial z}B(y,z)\right). \end{aligned}$$

(2) Next, we apply Jacobi's formula for the derivative of a determinant [14, part three, section A.3] to the matrix

$$M(y,z)=\begin{pmatrix} c_0 & -z & 0 & \cdots & 0 & -z \\ -z & c_1 & -z & \cdots & 0 & 0 \\ 0 & -z & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} & -z \\ -z & 0 & 0 & \cdots & -z & c_{q-1} \end{pmatrix}$$

to obtain

$$\frac{\partial}{\partial z}B(y,\,z)=\frac{\partial}{\partial z}\det(M(y,\,z))=\mathrm{tr}\left(\mathrm{adj}(M(y,\,z))\frac{\partial M(y,\,z)}{\partial z}\right).$$

This gives us, with I_q denoting the $q\times q$ identity matrix,

$$\begin{aligned}B(y,\,z)-\frac{z}{q}\frac{\partial}{\partial z}B(y,\,z)&=\det(M(y,\,z))-\frac{z}{q}\mathrm{tr}\left(\mathrm{adj}(M(y,\,z))\frac{\partial M(y,\,z)}{\partial z}\right)\\&=\frac{1}{q}\mathrm{tr}(\det(M(y,\,z))I_q)-\frac{z}{q}\mathrm{tr}\left(\mathrm{adj}(M(y,\,z))\frac{\partial M(y,\,z)}{\partial z}\right)\\&=\frac{1}{q}\mathrm{tr}(\mathrm{adj}(M(y,\,z))M(y,\,z))-\frac{z}{q}\mathrm{tr}\left(\mathrm{adj}(M(y,\,z))\frac{\partial M(y,\,z)}{\partial z}\right)\\&=\frac{1}{q}\mathrm{tr}\left(\mathrm{adj}(M(y,\,z))\left(M(y,\,z)-\frac{z}{q}\frac{\partial M(y,\,z)}{\partial z}\right)\right)\\&=\frac{1}{q}\mathrm{tr}(\mathrm{adj}(M(y,\,z))I_q)\\&=\frac{1}{q}\mathrm{tr}(\mathrm{adj}(M(y,\,z))).\end{aligned}$$

(3) The trace in this formula is the sum of q minors of $M(y,\,z)$, namely the determinants of the matrices obtained from $M(y,\,z)$ by removing a row and the corresponding column. Let these matrices be denoted $M_1(y,\,z)$, $M_2(y,\,z),\ldots,M_q(y,\,z)$. We note that $M_k(y,\,z)$ can be obtained from $M_1(y,\,z)$ by the substitution $y\mapsto Q^{k-1}y$ and cyclic permutation of rows and columns. It follows that

$$[y^0]M_1(y,\,z)=[y^0]M_2(y,\,z)=\cdots=[y^0]M_q(y,\,z),$$

so

$$\begin{aligned}b_{p/q}(z)-\frac{z}{q}b'_{p/q}(z)&=[y^0]\left(B(y,\,z)-\frac{z}{q}\frac{\partial}{\partial z}B(y,\,z)\right)\\&=[y^0]\frac{1}{q}(M_1(y,\,z)+M_2(y,\,z)+\cdots+M_q(y,\,z))\\&=[y^0]M_1(y,\,z).\end{aligned}$$

(4) On the other hand, if we expand the determinant

$$\begin{vmatrix}1&-z/x&0&\cdots&0&-zx\\1&c_1&-z/x&\cdots&0&0\\1&-zx&c_2&\cdots&0&0\\\vdots&\vdots&\vdots&\ddots&\vdots&\vdots\\1&0&0&\cdots&c_{q-2}&-z/x\\1&0&0&\cdots&-zx&c_{q-1}\end{vmatrix}$$

first with respect to the first column, then with respect to the first row, we obtain

$$\begin{vmatrix} c_1 & -z/x & \cdots & 0 & 0 \\ -zx & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{q-2} & -z/x \\ 0 & 0 & \cdots & -zx & c_{q-1} \end{vmatrix}$$

$$+\sum_{r=1}^{q-1}\frac{z^r}{x^r}\begin{vmatrix} c_{r+1} & -z/x & \cdots & 0 & 0 \\ -zx & c_{r+2} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{q-2} & -z/x \\ 0 & 0 & \cdots & -zx & c_{q-1} \end{vmatrix}$$

$$+\sum_{r=1}^{q-1} z^r x^r \begin{vmatrix} c_1 & -z/x & \cdots & 0 & 0 \\ -zx & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{q-r-2} & -z/x \\ 0 & 0 & \cdots & -zx & c_{q-r-1} \end{vmatrix}, \tag{27}$$

where an empty determinant is to be interpreted as 1. Now, we make use of the prior observation (see (11)) that determinants of the form

$$D_k = \begin{vmatrix} u_1 & -x_2 & \cdots & 0 & 0 \\ -x_1 & u_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & u_{k-1} & -x_2 \\ 0 & 0 & \cdots & -x_1 & u_k \end{vmatrix},$$

where the u_j are arbitrary coefficients, satisfy the recursion $D_k = u_k D_{k-1} - x_1 x_2 D_{k-2}$. Here, this implies that all the determinants in (27) are actually independent of x, so

$$[x^0y^0]\begin{vmatrix} 1 & -z/x & 0 & \cdots & 0 & -zx \\ 1 & c_1 & -z/x & \cdots & 0 & 0 \\ 1 & -zx & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & c_{q-2} & -z/x \\ 1 & 0 & 0 & \cdots & -zx & c_{q-1} \end{vmatrix}$$

$$= [x^0y^0]\begin{vmatrix} c_1 & -z/x & \cdots & 0 & 0 \\ -zx & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{q-2} & -z/x \\ 0 & 0 & \cdots & -zx & c_{q-1} \end{vmatrix} = [y^0]\begin{vmatrix} c_1 & -z & \cdots & 0 & 0 \\ -z & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{q-2} & -z \\ 0 & 0 & \cdots & -z & c_{q-1} \end{vmatrix}$$

$$= [y^0]M_1(y, z) = b_{p/q}(z) - \frac{z}{q}b'_{p/q}(z),$$

completing the proof of (18).

A.2. The Kreft coefficients

In (22) the coefficients $a_{p/q}(2i)$ are properly defined when $q \geqslant 2i$: one has

$$
\begin{aligned}
&a_{p/q}(0) = -1,\\
&a_{p/q}(2) = \sum_{i_1=0}^{q-2} 4\sin^2\left(\frac{\pi(i_1+1)p}{q}\right),\\
&a_{p/q}(4) = -\sum_{i_1=0}^{q-4}\sum_{i_2=0}^{i_1} 4\sin^2\left(\frac{\pi(i_1+3)p}{q}\right)4\sin^2\left(\frac{\pi(i_2+1)p}{q}\right),\\
&a_{p/q}(6) = \sum_{i_1=0}^{q-6}\sum_{i_2=0}^{i_1}\sum_{i_3=0}^{i_2} 4\sin^2\left(\frac{\pi(i_1+5)p}{q}\right)4\sin^2\left(\frac{\pi(i_2+3)p}{q}\right)4\sin^2\left(\frac{\pi(i_3+1)p}{q}\right),
\end{aligned}
$$

etc. One obtains in this way that

$$
\begin{aligned}
&a_{p/q}(2) = 2q,\\
&a_{p/q}(4) = -2q^2+7q+2q\cos\left(\frac{2\pi p}{q}\right),\\
&a_{p/q}(6) = \frac{4q^3-42q^2+116q}{3} + (-4q^2+24q)\cos\left(\frac{2\pi p}{q}\right) + 4q\cos\left(\frac{4\pi p}{q}\right),\\
&a_{p/q}(8) = \frac{-4q^4+84q^3-617q^2+1617q}{6} + (4q^3-62q^2+252q)\cos\left(\frac{2\pi p}{q}\right)\\
&\qquad + (-9q^2+77q)\cos\left(\frac{4\pi p}{q}\right) + 12q\cos\left(\frac{6\pi p}{q}\right) + 2q\cos\left(\frac{8\pi p}{q}\right),\\
&a_{p/q}(10) = \frac{4q^5-140q^4+1925q^3-12505q^2+32916q}{15}\\
&\qquad + \frac{-8q^4+228q^3-2260q^2+7896q}{3}\cos\left(\frac{2\pi p}{q}\right)\\
&\qquad + (10q^3-206q^2+1108q)\cos\left(\frac{4\pi p}{q}\right) + (-28q^2+312q)\cos\left(\frac{6\pi p}{q}\right)\\
&\qquad + (-4q^2+84q)\cos\left(\frac{8\pi p}{q}\right) + 16q\cos\left(\frac{10\pi p}{q}\right) + 4q\cos\left(\frac{12\pi p}{q}\right),
\end{aligned}
$$

etc.

A.3. Proof of the trace formula (24)

Let us return to the representation (19):

$$
\sum_{n\geqslant 0} Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q})z^n = \left(1-\frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\right)\sum_{k\geqslant 0}\binom{2k}{k}^2\left(\frac{z^q}{b_{p/q}(z)}\right)^{2k}.
$$

We notice first that

$$1 - \frac{z b'_{p/q}(z)}{q b_{p/q}(z)} = \frac{z}{q} \cdot \frac{\frac{\mathrm{d}}{\mathrm{d}z}\frac{z^q}{b_{p/q}(z)}}{\frac{z^q}{b_{p/q}(z)}},$$

so this can also be rewritten as

$$\begin{aligned}\sum_{n\geqslant 0} Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q}) z^n &= \frac{z}{q}\sum_{k\geqslant 0}\binom{2k}{k}^2\left(\frac{z^q}{b_{p/q}(z)}\right)^{2k-1}\frac{\mathrm{d}}{\mathrm{d}z}\frac{z^q}{b_{p/q}(z)}\\ &= \frac{z}{q}\frac{\mathrm{d}}{\mathrm{d}z}\left(\log\left(\frac{z^q}{b_{p/q}(z)}\right) + \sum_{k\geqslant 1}\binom{2k}{k}^2\frac{1}{2k}\left(\frac{z^q}{b_{p/q}(z)}\right)^{2k}\right).\end{aligned}$$

It follows that

$$Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q}) = \frac{n}{q}[z^n]\left(\log\left(\frac{z^q}{b_{p/q}(z)}\right) + \sum_{k\geqslant 1}\binom{2k}{k}^2\frac{1}{2k}\left(\frac{z^q}{b_{p/q}(z)}\right)^{2k}\right).$$

Now, set $s_{p/q}(z) = 1 - b_{p/q}(z) = \sum_{i=1}^{\lfloor q/2\rfloor} a(2i) z^{2i}$ and let us expand $-\log(b_{p/q}(z)) = -\log(1 - s_{p/q}(z))$ and $b_{p/q}(z)^{-2k} = (1 - s_{p/q}(z))^{-2k}$ into series. Note also that $\log(z^q) = q\log z$ does not contribute to the coefficient of z^n. We obtain

$$\begin{aligned}Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q}) &= \frac{n}{q}[z^n]\left(-\log(1 - s_{p/q}(z)) + \sum_{k\geqslant 1}\binom{2k}{k}^2\frac{z^{2kq}}{2k}(1 - s_{p/q}(z))^{2k}\right)\\ &= \frac{n}{q}[z^n]\left(\sum_{m\geqslant 1}\frac{s_{p/q}(z)^m}{m} + \sum_{k\geqslant 1}\binom{2k}{k}^2\frac{z^{2kq}}{2k}\sum_{m\geqslant 0}\binom{m+2k-1}{2k-1}s_{p/q}(z)^m\right).\end{aligned}$$

The two sums can be combined to a single one:

$$\begin{aligned}Z_n(\mathrm{e}^{2\mathrm{i}\pi p/q}) &= \frac{n}{q}[z^n]\sum_{\substack{k,m\geqslant 0\\(k,m)\neq(0,0)}}\frac{\binom{2k}{k}^2\left(\frac{m+2k}{2k}\right)}{m+2k}z^{2kq}s_{p/q}(z)^m = \frac{n}{q}\\ &\quad\times\sum_{\substack{k,m\geqslant 0\\(k,m)\neq(0,0)}}\frac{\binom{2k}{k}^2\left(\frac{m+2k}{2k}\right)}{m+2k}[z^{n-2kq}]s_{p/q}(z)^m. \qquad (28)\end{aligned}$$

When $s_{p/q}(z)^m = \left(\sum_{i=1}^{\lfloor q/2\rfloor} a(2i) z^{2i}\right)^m$ is expanded, the resulting terms are of the form

$$\binom{m}{\ell_1, \ell_2, \ldots, \ell_{\lfloor q/2\rfloor}} z^{2(\ell_1 + 2\ell_2 + \cdots + \lfloor q/2\rfloor \ell_{\lfloor q/2\rfloor})}\prod_{j=1}^{\lfloor q/2\rfloor} a(2j)^{\ell_j},$$

where $\ell_1 + \ell_2 + \cdots + \ell_{\lfloor q/2\rfloor} = m$. Since we are taking the coefficient of z^{n-2kq}, the ℓ_j have to satisfy

$$\ell_1 + 2\ell_2 + \cdots + \lfloor q/2\rfloor \ell_{\lfloor q/2\rfloor} = n/2 - kq.$$

Putting everything together, we arrive at (24). Note that $k = m = 0$ is impossible for $n > 0$, so the restriction in the sum (28) is actually immaterial.

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Chapter

3 Hofstadter point spectrum trace and the almost Mathieu operator

In this Chapter, we introduce another method to rederive the main results of chapter 2, i.e eq. (2.23):

$$\mathrm{Tr}H^n_{2\pi p/q} = \frac{n}{q}\sum_{k\geq 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-kq}} \frac{\binom{2k}{k}^2\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}\prod_{j=1}^{\lfloor q/2\rfloor} a_{p/q}(2j)^{\ell_j}$$

and eq. (2.22):

$$\sum_{n\geq 0}\mathrm{Tr}H^n_{2\pi p/q}z^n = \Big(1-\frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\Big)\frac{2}{\pi}K\Big(\frac{16z^{2q}}{b_{p/q}(z)^2}\Big).$$

in the quantum mechanics formalism. We will focus in the Hofstadter model on the so called "point spectrum traces". The main results have been published in [13], which is inserted at the end of this chapter (Article 2).

In order to achieve this goal, we start in section 3.1 by some general considerations on how to calculate $\mathrm{Tr}H^n_{2\pi p/q}$, the trace of the n-th moment Hofstadter Hamiltonian. In section 3.2, we will introduce what a "point spectrum trace" is and how to use it to recover the full trace of the Hofstadter Hamiltonian. In section 3.3, we will show this procedure can be extended to the asymmetric case without too much difficulty, allowing for a trace formula expressed in terms of the generalized Kreft coefficients for the almost Mathieu operator.

3.1 Introduction and reminder of the Hofstadter model

Recall the Hamiltonian of the Hofstadter model

$$H_\gamma = T_x + T_x^{-1} + T_y + T_y^{-1} \tag{3.1}$$

with $T_xT_y = \exp(-i\gamma)\,T_yT_x$. Its eigenvalue equation is the Harper's equation

$$\Phi_{m+1} + \Phi_{m-1} + 2\cos(k_y+\gamma m)\Phi_m = E\Phi_m. \tag{3.2}$$

In the commensurate case with a rational flux $\gamma = 2\pi p/q$, p and q coprimes, it follows a q-periodic condition of the wavefunction: $\Phi_{m+q} = e^{iqk_x}\Phi_m$. The eigenvalue equation reduces to a $q \times q$ matrix $m_{p/q}(E, k_x, k_y)$ (k_x and k_y are wave numbers $\in [-\pi, \pi]$) acting with zero output on the q-components eigenvector $\{\Phi_0, \Phi_1, \ldots \Phi_{q-1}\}$:

$$\begin{pmatrix} 2\cos(k_y) - E & 1 & 0 & \cdots & 0 & e^{-iqk_x} \\ 1 & 2\cos\Big(k_y + \frac{2\pi p}{q}\Big) - E & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ e^{iqk_x} & 0 & 0 & \cdots & 1 & 2\cos\Big(k_y + (q-1)\frac{2\pi p}{q}\Big) - E \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{q-2} \\ \Phi_{q-1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}. \tag{3.3}$$

Hence, the q eigenenergies $E_r(k_x, k_y)$ with $r = 1, 2, \ldots, q$ are the roots of the secular equation

$$\det\big(m_{p/q}(E, k_x, k_y)\big) = 0. \tag{3.4}$$

The trace of the n-th moment Hofstadter Hamiltonian is defined as

$$\text{Tr } H^n_{2\pi p/q} = \frac{1}{q}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\sum_{r=1}^{q} E_r^n(k_x, k_y), \tag{3.5}$$

where the integrations are over the quasi-momenta k_x and $k_y \in [-\pi, \pi]$. As mentioned in Article 1, evaluating Tr $H^n_{2\pi p/q}$ in this way is involved, because each of the q eigenenergies $E_r\,(k_x, k_y)$ depends on k_x and k_y, plus, k_x and k_y vary continuously in the interval $\in [-\pi, \pi]$. Fortunately, there exists a very elegant identity for the determinant $\det\big(m_{p/q}(E, k_x, k_y)\big)$ which is the Chambers identity [17]

$$\det\big(m_{p/q}(E, k_x, k_y)\big) = \det\big(m_{p/q}(E, 0, 0)\big) + 4(-1)^q - 2(-1)^q\left(\cos(qk_x) + \cos(qk_y)\right) \tag{3.6}$$

This identity says that the $\det\big(m_{p/q}(E, k_x, k_y)\big)$ decomposes into two part: the first part $\det\big(m_{p/q}(E, 0, 0)\big) + 4(-1)^q$ is the characteristic polynomial of E with degree q which is independent of k_x and k_y; the second part is composed by $\cos(qk_x)$ and $\cos(qk_y)$. We define the characteristic polynomial as

$$\det\big(m_{p/q}(E, 0, 0)\big) + 4(-1)^q = (-1)^q E^q b_{p/q}(1/E) \tag{3.7}$$

with $b_{p/q}(z)$ is a polynomial with degree $2[\frac{q}{2}]$ (2 times the integer part of $q/2$)

$$b_{p/q}(z) = -\sum_{i=0}^{[\frac{q}{2}]} a_{p/q}(2i) z^{2i} \tag{3.8}$$

in terms of the Kreft coefficients $a_{p/q}(2i)$

$$a_{p/q}(2i) = (-1)^{i+1}\sum_{k_1=0}^{q-2i}\sum_{k_2=0}^{k_1}\cdots\sum_{k_i=0}^{k_{i-1}} 4\sin^2\left(\frac{\pi(k_1 + 2i - 1)p}{q}\right) 4\sin^2\left(\frac{\pi(k_2 + 2i - 3)p}{q}\right)\ldots 4\sin^2\left(\frac{\pi(k_i + 1)p}{q}\right)$$

as mentioned in eq. (2.18) chapter 2. Note that $a_{p/q}(2i) = 0$ as soon as $q < 2i$. How to derive these coefficients is explained in Kreft's paper [15] (see the Appendix A for details). Therefore, eq. (3.4) becomes

$$E^q b_{p/q}(1/E) = 2\left(\cos\left(qk_x\right) + \cos\left(qk_y\right)\right). \tag{3.9}$$

Solving eq. (3.4) leads to consider

$$E^q b_{p/q}(1/E) = \pm s \tag{3.10}$$

where s varies in $[0, 4]$ since $2\left(\cos(qk_x) + \cos(qk_y)\right)$ varies in $[-4, 4]$. We denote $E_r(\pm s)$ as the roots of eq. (3.10). $E^q b_{p/q}(1/E)$ has the following properties (see the figure 1 and the figure 2 in Article 2):

- (i) $E^q b_{p/q}(1/E)$ is a polynomial of degree q, therefore for a given $\gamma = 2\pi p/q$, there are q energy bands, and each band never overlap each other except for the case q even, the two central bands kiss each other in zero energy (see P. Van Mouche [18]).
- (ii) $E^q b_{p/q}(1/E)$ is lying between -4 and 4. In fact, the eigenenergies also vary within the interval $[-4, 4]$ (see the proof in the Appendix C).
- (iii) There exist some symmetry properties of $E_r(s)$ and $E_r(-s)$: when q is odd, $E_r(s) = -E_{q+1-r}(-s)$; when q is even, $E_r(\pm s) = -E_{q+1-r}(\pm s)$.

We consider the point spectrum traces

$$\mathrm{Tr}_{\pm \mathrm{s}} H^n_{2\pi p/q} = \frac{1}{2q}\sum_{r=1}^{q}\Big(E^n_r(s) + E^n_r(-s)\Big) \tag{3.11}$$

To recover the full quantum Hofstadter trace, we will argue that it will be sufficient to do an integration of $\mathrm{Tr}_{\pm \mathrm{s}} H^n_{2\pi p/q}$ over $s \in [-4, 4]$ with an appropriate density of state $\rho(s)$ such that

$$\int_{-4}^{4} \mathrm{Tr}_{\pm \mathrm{s}} H^n_{2\pi p/q}\rho(s)ds = \mathrm{Tr} H^n_{2\pi p/q}. \tag{3.12}$$

In the next section, we will show how to calculate the point spectrum trace $\mathrm{Tr}_{\pm \mathrm{s}} H^n_{2\pi p/q}$ and what is the appropriate density of state $\rho(s)$ to recover the full quantum Hofstadter trace.

3.2 Point spectrum trace formula and density of states

3.2.1 $\pm s$ trace formula:

In this section, we consider how to calculate the point spectrum trace

$$\mathrm{Tr}_{\pm \mathrm{s}} H^n_{2\pi p/q} = \frac{1}{2q}\sum_{r=1}^{q}\Big(E^n_r(s) + E^n_r(-s)\Big).$$

We define the generating function of $\mathrm{Tr}_{\pm \mathrm{s}} H^n_{2\pi p/q}$ such that

$$\begin{aligned}
\sum_{n\geq 0, n \text{ even}} \mathrm{Tr}_{\pm \mathrm{s}} H^n_{2\pi p/q} z^n &= \sum_{n\geq 0}\frac{1}{2q}\Big(\sum_{r=1}^{q} E^n_r(s) + \sum_{r=1}^{q} E^n_r(-s)\Big) z^n \\
&= \frac{1}{2q}\Big(\sum_{r=1}^{q}\sum_{n\geq 0}(zE_r(s))^n + \sum_{r=1}^{q}\sum_{n\geq 0}(zE_r(-s))^n\Big) \\
&= \frac{1}{2q}\Big(\sum_{r=1}^{q}\frac{1}{1 - zE_r(s)} + \sum_{r=1}^{q}\frac{1}{1 - zE_r(-s)}\Big),
\end{aligned}$$

On the other hand, since the $E_r(s)$'s are the root of $E_r^q(s)b_{p/q}(1/E(s)) = s$, we have

$$(1/z)^q b_{p/q}(z) - s = \prod_{r=1}^{q}(1/z - E_r(s)),$$

which is equivalent to

$$b_{p/q}(z) - sz^q = \prod_{r=1}^{q}(1 - zE_r(s)),$$

so that

$$\big(\log\big(b_{p/q}(z)\big)\big)' = \sum_{r=1}^{q}\frac{-E_r(s)}{1-zE_r(s)} = \frac{1}{z}\sum_{r=1}^{q}\Big(1 - \frac{1}{1-zE_r(s)}\Big)$$

which is the same as

$$\frac{\big(b_{p/q}(z) - sz^q\big)'}{\big(b_{p/q}(z) - sz^q\big)} = \frac{1}{z}\Big(q - \sum_{r=1}^{q}\frac{1}{1-zE_r(s)}\Big).$$

With the substitutions above, the s spectrum trace generating function becomes

$$\begin{aligned}\sum_{n\geq 0}\mathrm{Tr}_{\pm\mathrm{s}}H^n_{2\pi p/q}z^n &= 1 - \frac{z\big(b_{p/q}(z) - sz^q\big)'}{2q\big(b_{p/q}(z) - sz^q\big)} - \frac{z\big(b_{p/q}(z) + sz^q\big)'}{2q\big(b_{p/q}(z) + sz^q\big)}\\ &= \Big(1 - \frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\Big)\frac{1}{1 - s^2(\frac{z^q}{b_{p/q}(z)})^2}. \end{aligned} \tag{3.13}$$

It should be noted that n is always even because of the symmetric properties of $E_r(s)$ (as mentioned in section 3.1), which is in correspondence with closed random walks, where the total number of steps must be even.

In order to find the explicit formula for $\mathrm{Tr}_{\pm\mathrm{s}}H^n_{2\pi p/q}$, we rewrite its generating function as

$$\begin{aligned}\sum_{n\geq 0}\mathrm{Tr}_{\pm\mathrm{s}}H^n_{2\pi p/q}z^n &= \frac{z}{q}\cdot\frac{\frac{d}{dz}\frac{z^q}{b_{p/q}(z)}}{\frac{z^q}{b_{p/q}(z)}}\frac{1}{1 - s^2(\frac{z^q}{b_{p/q}(z)})^2}\\ &= \frac{z}{q}\sum_{k\geq 0}\Big(s^{2k}\frac{z^q}{b_{p/q}(z)}\Big)^{2k-1}\frac{d}{dz}\frac{z^q}{b_{p/q}(z)}\\ &= \frac{z}{q}\frac{d}{dz}\bigg(\log\Big(\frac{z^q}{b_{p/q}(z)}\Big) + \sum_{k\geq 1}\frac{s^{2k}}{2k}\Big(\frac{z^q}{b_{p/q}(z)}\Big)^{2k}\bigg).\end{aligned}$$

It follows that the $\mathrm{Tr}_{\pm\mathrm{s}}H^n_{2\pi p/q}$ is just the coefficient of z^n of $\sum_{n\geq 0}\mathrm{Tr}_{\pm\mathrm{s}}H^n_{2\pi p/q}z^n$:

$$\mathrm{Tr}_{\pm\mathrm{s}}H^n_{2\pi p/q} = [z^n]\bigg(\log\Big(\frac{z^q}{b_{p/q}(z)}\Big) + \sum_{k\geq 1}\frac{s^{2k}}{2k}\Big(\frac{z^q}{b_{p/q}(z)}\Big)^{2k}\bigg).$$

Now set $v_{p/q}(z) = 1 - b_{p/q}(z) = \sum_{i=1}^{\lfloor q/2\rfloor}a(2i)z^{2i}$ and let us expand $-\log\big(b_{p/q}(z)\big) = -\log\big(1 - v_{p/q}(z)\big)$ and $b_{p/q}(z)^{-2k} = (1 - v_{p/q}(z))^{-2k}$ into series. Note also that $\log(z^q) = q\log z$ does not contribute to the coefficient of z^n. We obtain

$$\begin{aligned}\mathrm{Tr}_{\pm\mathrm{s}}H^n_{2\pi p/q} &= \frac{n}{q}[z^n]\bigg(-\log\big(1 - v_{p/q}(z)\big) + \sum_{k\geq 1}\frac{(sz^q)^{2k}}{2k}(1 - v_{p/q}(z))^{2k}\bigg)\\ &= \frac{n}{q}[z^n]\bigg(\sum_{m\geq 1}\frac{v_{p/q}(z)^m}{m} + \sum_{k\geq 1}\frac{(sz^q)^{2k}}{2k}\sum_{m\geq 0}\binom{m+2k-1}{2k-1}v_{p/q}(z)^m\bigg).\end{aligned}$$

The two sums can be combined in a single one:

$$\mathrm{Tr}_{\pm s} H^n_{2\pi p/q} = \frac{n}{q}[z^n] \sum_{\substack{k,m\geq 0\\(k,m)\neq(0,0)}} \frac{s^{2k}\binom{m+2k}{2k}}{m+2k} z^{2kq} v_{p/q}(z)^m = \frac{n}{q} \sum_{\substack{k,m\geq 0\\(k,m)\neq(0,0)}} \frac{s^{2k}\binom{m+2k}{2k}}{m+2k} [z^{n-2kq}] v_{p/q}(z)^m. \tag{3.14}$$

When $v_{p/q}(z)^m = \left(\sum_{i=1}^{\lfloor q/2\rfloor} a(2i) z^{2i}\right)^m$ is expanded, the resulting terms are of the form

$$\binom{m}{\ell_1, \ell_2, \ldots, \ell_{\lfloor q/2\rfloor}} z^{2(\ell_1 + 2\ell_2 + \cdots + \lfloor q/2\rfloor \ell_{\lfloor q/2\rfloor})} \prod_{j=1}^{\lfloor q/2\rfloor} a(2j)^{\ell_j},$$

where $\ell_1 + \ell_2 + \cdots + \ell_{\lfloor q/2\rfloor} = m$. Since we are taking the coefficient of z^{n-2kq}, the ℓ_j have to satisfy

$$\ell_1 + 2\ell_2 + \cdots + \lfloor q/2\rfloor \ell_{\lfloor q/2\rfloor} = n/2 - kq.$$

Putting everything together, we arrive an explicit sum formula for the point spectrum trace

$$\mathrm{Tr}_{\pm s} H^n_{2\pi p/q} = \frac{n}{q} \sum_{k\geq 0} \sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor \ell_{\lfloor q/2\rfloor} = n/2-qk}} \frac{\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k} s^{2k} \prod_{j=1}^{\lfloor q/2\rfloor} a_{p/q}(2j)^{\ell_j} \tag{3.15}$$

Note that $k = m = 0$ is impossible for $n > 0$, so the restriction in the sum eq. (3.14) is actually immaterial.

Another thing to keep in mind is that comparing the Hofstadter trace eq. (2.23) with the point spectrum trace eq. (3.15), we remark that they coincide when $q > n/2$ since then the summation index k in eq. (3.15) necessarily vanishes. It means that $\mathrm{Tr}_{\pm s} H^n_{2\pi p/q}$ is independent of s as soon as $q > n/2$. In Arcticle 2, we also gave the formula for a particular case of the point spectrum trace where $s = 0$, the mid-band trace $\mathrm{Tr}_0 H^n_{2\pi p/q}$. A qualitative interpretation for these traces can stem from the classical picture of lattice walks contained in the periodic quantum cell of horizontal length q (the lattice walk the farthest on the horizontal axis from the origin indeed goes to a distance $n/2$).

3.2.2 Density of states:

Now, in order to recover the full Hofstadter quantum trace $\mathrm{Tr} H^n_{2\pi p/q}$, one has to find a suitable density of the states such that

$$\int_{-4}^{4} \mathrm{Tr}_{\pm s} H^n_{2\pi p/q} \rho(s) ds = \mathrm{Tr} H^n_{2\pi p/q}. \tag{3.16}$$

and by comparing the full Hofstadter quantum trace $\mathrm{Tr} H^n_{2\pi p/q}$ eq. (2.23) with the $\pm s$ point spectrum trace $\mathrm{Tr}_{\pm s} H^n_{2\pi p/q}$ eq. (3.15), the density of states $\rho(s)$ should satisfy the condition

$$\int_{-4}^{4} s^{2k} \rho(s) ds = \binom{2k}{k}^2 \tag{3.17}$$

then,

$$\rho(s) = 1/(2\pi^2) K(1 - s^2/16), \tag{3.18}$$

it is the density of states for the free spectrum $s = 2(\cos(qk_x) + \cos(qk_y))$. For more details about this density, please see the section III.C of Article 2.

3.3 $\lambda \neq 2$: almost Mathieu operator

The methods used above can be extended to the more general case of the almost Mathieu operator [5],

$$\Phi_{m+1} + \Phi_{m-1} + \lambda \cos(k_y + \gamma m)\Phi_m = E\Phi_m \tag{3.19}$$

which is similar to the Mathieu equation :

$$-y''(x) + \lambda \cos(x)y(x) = Ey(x). \tag{3.20}$$

The equation eq. (3.19) is a one-dimensional discrete Schrödinger equation, which can be understood as a tight binding model for the Hamiltonian of a single electron in a rectangular lattice coupled with a perpendicular magnetic field. It introduces a new variable λ who corresponds to the ratio between the vertical and the horizontal hopping amplitudes. In the Hofstadter case, $\lambda/2 = 1$ because of the symmetry of movement between horizontal and vertical direction. In section 3.2, we recovered the full quantum Hofstadter trace $\mathrm{Tr}H^n_{2\pi p/q}$ by integrating point spectrum traces $\mathrm{Tr}_{\pm \mathrm{s}}H^n_{2\pi p/q}$ with the appropriate free density of states $\rho(s)$ on the lattice. This construction can be generalized to the almost Mathieu operator when $\gamma = 2\pi p/q$ with p and q are coprime integers. We can calculate the n-th moment trace formula for the almost Mathieu operator $\mathrm{Tr}\left(H^{(\lambda)}_{2\pi p/q}\right)^n$ in terms of the generalized Kreft coefficients $a^{(\lambda)}_{p/q}(2j)$ which depend on λ. Indeed, in the Hofstadter case, when $\gamma = 2\pi p/q$, eq. (3.19) can reduce to a $q \times q$ secular matrix

$$m^{(\lambda)}_{p/q}(E, k_x, k_y) = \begin{pmatrix} \lambda\cos(k_y) - E & 1 & 0 & \cdots & 0 & e^{-iqk_x} \\ 1 & \lambda\cos\left(k_y + \frac{2\pi p}{q}\right) - E & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ e^{iqk_x} & 0 & 0 & \cdots & 1 & \lambda\cos\left(k_y + (q-1)\frac{2\pi p}{q}\right) - E \end{pmatrix}. \tag{3.21}$$

The generalized Chamber's identity is then

$$\det\left(m^{(\lambda)}_{p/q}(E, k_x, k_y)\right) = \det\left(m^{(\lambda)}_{p/q}(E, 0, 0)\right) - 2(-1)^q(\cos(qk_x) - 1 + (\lambda/2)^q(\cos(qk_y) - 1)). \tag{3.22}$$

The eigenvalue equation becomes

$$\det\left(m^{(\lambda)}_{p/q}(E, 0, 0)\right) = 2(-1)^q(\cos(qk_x) - 1 + (\lambda/2)^q(\cos(qk_y) - 1)). \tag{3.23}$$

In Article 2, we introduce the polynomial $b^{(\lambda)}_{p/q}(z)$

$$b^{(\lambda)}_{p/q}(z) = -\sum_{j=0}^{[\frac{q}{2}]} a^{(\lambda)}_{p/q}(2j)z^{2j} \tag{3.24}$$

with the generalized Kreft coefficients $-a^{(\lambda)}_{p/q}(2j)$ (with $a^{(\lambda)}_{p/q}(0) = -1$)

$$\begin{aligned} a^{(\lambda)}_{p/q}(2j) \;=\; & (-1)^{j+1} \sum_{k_1=0}^{q-2j} \sum_{k_2=0}^{k_1} \cdots \sum_{k_j=0}^{k_{j-1}} \alpha^{(\lambda)}_{p/q}(k_1 + 2j - 2)\overline{\alpha}^{(\lambda)}_{p/q}(k_1 + 2j - 2) \\ & \alpha^{(\lambda)}_{p/q}(k_2 + 2j - 4)\overline{\alpha}^{(\lambda)}_{p/q}(k_2 + 2j - 4) \ldots \alpha^{(\lambda)}_{p/q}(k_j)\overline{\alpha}^{(\lambda)}_{p/q}(k_j) \end{aligned} \tag{3.25}$$

where

$$\alpha^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{-ik_y}\left(1 - e^{\frac{2i\pi(k+1)p}{q}}\right) \text{ and } \overline{\alpha}^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{ik_y}\left(1 - (2/\lambda)^2 e^{-\frac{2i\pi(k+1)p}{q}}\right).$$

Appendix A shows the detailed derivation of the generalized Kreft coefficients $a^{(\lambda)}_{p/q}(2i)$. With the substitutions above, $\det\Big(m^{(\lambda)}_{p/q}(E,0,0)\Big)$ rewrites as

$$\det\Big(m^{(\lambda)}_{p/q}(E,0,0)\Big) + 2(-1)^q(1+(\lambda/2)^q) = (-1)^q E^q b^{(\lambda)}_{p/q}(1/E), \tag{3.26}$$

$\det\Big(m^{(\lambda)}_{p/q}(E,k_x,k_y)\Big)$ decomposes into two parts: $E^q b^{(\lambda)}_{p/q}(1/E)$, a polynomial of E and a trigonometric part independent of E. A proof of Chamber's identity is given in Appendix B. Then, the eigenvalue equation eq. (3.23) rewrites as

$$E^q b^{(\lambda)}_{p/q}(1/E) = 2(\cos(qk_x) + (\lambda/2)^q\cos(qk_y)) = \pm s. \tag{3.27}$$

with $0 \leq |s| \leq 2\big(1+(\lambda/2)^q\big)$ and $-(2+\lambda) \leq E \leq 2+\lambda$ with $\lambda \geq 0$ (see the proof in Appendix C, section $\lambda \neq 2$).

The almost Mathieu operator quantum trace, $\mathrm{Tr}\Big(H^{(\lambda)}_{2\pi p/q}\Big)^n$ is defined as

$$\mathrm{Tr}\,(H^{(\lambda)}_{2\pi p/q})^n = \frac{1}{q}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\sum_{r=1}^{q}(E^{(\lambda)}_r(k_x,k_y))^n, \tag{3.28}$$

where the $E^{(\lambda)}_r(k_x,k_y)$'s are the eigenvalues of eq. (3.27). Following the same logic as in the Hofstadter case, instead of calculating $\mathrm{Tr}\,(H^{(\lambda)}_{2\pi p/q})^n$ directly from eq. (3.28), we aim at the point spectrum traces $\mathrm{Tr_s}\Big(H^{(\lambda)}_{2\pi p/q}\Big)^n$ with the appropriate density of states $\rho^{(\lambda)}(s)$ such that

$$\int_{-2(1+(\lambda/2)^q)}^{2(1+(\lambda/2)^q)}\mathrm{Tr_s}(H^{(\lambda)}_{2\pi p/q})^n\rho^{(\lambda)}(s)ds = \mathrm{Tr}(H^{(\lambda)}_{2\pi p/q})^n.$$

The key point to obtain the point spectrum trace $\mathrm{Tr_s}\Big(H^{(\lambda)}_{2\pi p/q}\Big)^n$ and its generating function $\mathrm{Tr_s}\Big(H^{(\lambda)}_{2\pi p/q}\Big)^n z^n$ is to follow precisely the same steps as in section 3.2, which means we replace the $a_{p/q}(2j)$ by $a^{(\lambda)}_{p/q}(2j)$ in eq. (3.15) and eq. (3.13), replace the $b_{p/q}(z)$ by $b^{(\lambda)}_{p/q}(z)$ and derive the appropriate density $\rho^{(\lambda)}(s)$. For a more detailed derivation, please see the section IV. of Article 2. The results are the following

$$\begin{aligned}\mathrm{Tr}\,(H^{(\lambda)}_{2\pi p/q})^n =& \frac{n}{q}\sum_{k\geq 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-qk}}\frac{\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}\binom{2k}{k}\sum_{k_1=0}^{k}\binom{k}{k_1}^2(\lambda/2)^{2qk_1}\\ &\prod_{j=1}^{\lfloor q/2\rfloor}a^{(\lambda)}_{p/q}(2j)^{\ell_j},\end{aligned} \tag{3.29}$$

which is a λ-deformation of the quantum Hofstadter trace eq. (2.23).

One also gets the generating function that generalizes eq. (2.22)

$$\sum_{n\geq 0}\mathrm{Tr}\,\Big(H^{(\lambda)}_{2\pi p/q}\Big)^n z^n = \Big(1-\frac{z\big(b^{(\lambda)}_{p/q}(z)\big)'}{qb^{(\lambda)}_{p/q}(z)}\Big)\sum_{k\geq 0}\binom{2k}{k}\sum_{k_1=0}^{k}\binom{k}{k_1}^2(\lambda/2)^{2qk_1}\Big(\frac{z^q}{b^{(\lambda)}_{p/q}(z)}\Big)^{2k}, \tag{3.30}$$

which rewrites as

$$\sum_{n\geq 0}\mathrm{Tr}\,\Big(H^{(\lambda)}_{2\pi p/q}\Big)^n z^n = \Big(1-\frac{z\big(b^{(\lambda)}_{p/q}(z)\big)'}{qb^{(\lambda)}_{p/q}(z)}\Big)\frac{1}{\sqrt{1-4\big(\frac{z^q}{b^{(\lambda)}_{p/q}(z)}\big)^2\big(1-(\lambda/2)^q\big)^2}}\frac{2}{\pi}K\Big(\frac{16z^{2q}(\lambda/2)^q}{b^{(\lambda)}_{p/q}(z)^2-4z^{2q}\big(1-(\lambda/2)^q\big)^2}\Big) \tag{3.31}$$

It should be noted that the expression eq. (3.31) for the generating function can be obtained directly from eq. (3.28). The appendix E provides details on the derivation of it.

Another remark is that we can reproduce the results eq. (3.29) and eq. (3.30) from the lattice walks point of view as in chapter 2. Except that for the case $\lambda \neq 2$, the lattice is asymmetric (rectangular), so we denote $\lambda/2$ as the ratio between the horizontal axis and the vertical axis, then we consider the generating function $A(x_1, x_2, y_1, y_2, Q)$ (defined in eq. (2.9) of chapter 2), we replace x_1 by zx, x_2 by z/x, y_1 by $\lambda/2zy$ and $\lambda/2z/y$ and look at the coefficients with vanishing exponents in x and y and the exponent of n in z, which will in turn yield the generating function for the traces Tr $(H^{(\lambda)}_{2\pi p/q})^n$. For more details, please see the appendix C of Article 2.

By using our result eq. (3.29), in Article 2, we also checked that the Aubry-André duality [19] (it is an important property which relate eigenfunctions and spectra of the almost Mathieu operator with given λ to those of the almost Mathieu operator with λ replaced by $4/\lambda$)

$$\text{Tr } (H^{(\lambda)}_{2\pi p/q})^n = (\frac{\lambda}{2})^n \text{Tr } (H^{(4/\lambda)}_{2\pi p/q})^n, \tag{3.32}$$

holds, as it should.

3.4 Conclusion

In this chapter, we have introduced the point spectrum trace eq. (3.15) to recover the full Hofstadter quantum trace eq. (2.23). This procedure has been extended to the almost Mathieu operator in the commensurate case.

Article 2 : Hofstadter point spectrum trace and the almost Mathieu operator

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Hofstadter point spectrum trace and the almost Mathieu operator

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We consider point spectrum traces in the Hofstadter model. We show how to recover the full quantum Hofstadter trace by integrating these point spectrum traces with the appropriate free density of states on the lattice. This construction is then generalized to the almost Mathieu operator and its nth moments which can be expressed in terms of generalized Kreft coefficients. *Published by AIP Publishing.* https://doi.org/10.1063/1.5020147

I. INTRODUCTION

In Ref. 1, we focused on the algebraic area generating function of closed lattice walks of a given length n (n is then necessarily even),

$$Z_n(e^{i\gamma}),$$

evaluated at $e^{i\gamma}$, a root of unity. One reason for studying this quantity arises from the connection of the algebraic area distribution of random curves to the quantum spectrum of a charged particle in a perpendicular magnetic field. In the lattice case at hand, the mapping is on the quantum Hofstadter model[2] of a particle hopping on a two-dimensional lattice in a magnetic flux γ, counted in unit of the flux quantum. More precisely, $Z_n(e^{i\gamma})$ is mapped on the nth moment $\mathrm{Tr}\, H_\gamma^n$ of the Hofstadter Hamiltonian H_γ—thereafter referred to as the quantum Hofstadter trace—

$$Z_n(e^{i\gamma}) = \mathrm{Tr}\, H_\gamma^n$$

by virtue of which evaluating $Z_n(e^{i\gamma})$ for classical lattice walks gives an expression[1] for the Hofstadter quantum trace $\mathrm{Tr}\, H_\gamma^n$. In the simplified case of a rational flux, not surprisingly, the trace $\mathrm{Tr}\, H_\gamma^n$ can be written in terms of the Kreft coefficients[3] which encode the Schrödinger equation for the Hofstadter model

$$\Phi_{m+1} + \Phi_{m-1} + 2\cos(k_y + \gamma m)\Phi_m = E\Phi_m. \tag{1}$$

One would like to generalize this construction to the almost Mathieu operator case

$$\Phi_{m+1} + \Phi_{m-1} + \lambda\cos(k_y + \gamma m)\Phi_m = E\Phi_m, \tag{2}$$

where λ is now a free parameter. This operator, among other things, plays an important role in the characterization of the fractal structure of the Hofstadter spectrum.[4] Physically, it describes a quantum particle hopping on a lattice with horizontal and vertical amplitudes in a ratio λ.

We will first rederive the results of Ref. 1 by starting from point spectrum traces—to be defined later—and integrating them with the appropriate free density of states on the lattice in order to recover the quantum trace $\mathrm{Tr}\, H_\gamma^n$. This approach is original and gives a new light on the results obtained in Ref. 1. The generalization to the almost Mathieu case will then follow provided that one can extend accordingly the Kreft coefficients construction to the $\lambda \neq 2$ case. Finally we will discuss in Sec. V some direct links which can be established with current activities in the field.[10]

II. A REMINDER

In the commensurate case with a rational flux $\gamma = 2\pi p/q$, with p and q co-primes, the lattice Hofstadter eigenstates $\psi_{m,n} = e^{ink_y}\Phi_m$ are q-periodic on the horizontal axis $\Phi_{m+q} = e^{iqk_x}\Phi_m$. The Schrödinger equation (1) then reduces to a $q \times q$ secular matrix $m_{p/q}(E, k_x, k_y)$ acting with zero output on the q-components eigenvector $\{\Phi_0, \Phi_1, \ldots, \Phi_{q-1}\}$,

$$\begin{pmatrix} 2\cos(k_y) - E & 1 & 0 & \cdots & 0 & e^{-iqk_x} \\ 1 & 2\cos(k_y + \frac{2\pi p}{q}) - E & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ e^{iqk_x} & 0 & 0 & \cdots & 1 & 2\cos(k_y + (q-1)\frac{2\pi p}{q}) - E \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{q-2} \\ \Phi_{q-1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}. \tag{3}$$

The q eigenenergies $E_1(k_x, k_y)$, $E_2(k_x, k_y)$, …, $E_q(k_x, k_y)$ are the roots of $\det(m_{p/q}(E, k_x, k_y)) = 0$, which, thanks to the identity

$$\det(m_{p/q}(E, k_x, k_y)) = \det(m_{p/q}(E, 0, 0)) - 2(-1)^q(\cos(qk_x) - 1 + \cos(qk_y) - 1), \tag{4}$$

rewrites (see Ref. 5) as

$$\det(m_{p/q}(E, 0, 0)) = 2(-1)^q(\cos(qk_x) - 1 + \cos(qk_y) - 1). \tag{5}$$

The polynomial $b_{p/q}(z)$ with coefficients $-a_{p/q}(2j)$,

$$b_{p/q}(z) := -\sum_{j=0}^{[\frac{q}{2}]} a_{p/q}(2j) z^{2j}, \tag{6}$$

($a_{p/q}(0) = -1$) materializes in $\det(m_{p/q}(E, 0, 0))$ as

$$\det(m_{p/q}(E, 0, 0)) + 4(-1)^q = (-1)^q E^q b_{p/q}(1/E) \tag{7}$$

so that (5) becomes

$$E^q b_{p/q}(1/E) = 2(\cos(qk_x) + \cos(qk_y)). \tag{8}$$

The $a_{p/q}(2j)$'s in $b_{p/q}(z)$ in (6) are related to the Kreft coefficients $c_{p/q}(2j)$ as

$$\det(m_{p/q}(E, 0, 0)) + 4(-1)^q = \sum_{j=\frac{q}{2}-\lfloor\frac{q}{2}\rfloor}^{\frac{q}{2}} c_{p/q}(2j) E^{2j}$$

so that $a_{p/q}(2j) = c_{p/q}(q - 2j)(-1)^{q+1}$. One gets

$$a_{p/q}(2j) = (-1)^{j+1} \sum_{k_1=0}^{q-2j} \sum_{k_2=0}^{k_1} \cdots \sum_{k_j=0}^{k_{j-1}} 4\sin^2\left(\frac{\pi(k_1 + 2j - 1)p}{q}\right) 4\sin^2\left(\frac{\pi(k_2 + 2j - 3)p}{q}\right) \cdots \times 4\sin^2\left(\frac{\pi(k_j + 1)p}{q}\right), \tag{9}$$

with building blocks

$$4\sin^2\left(\frac{\pi(k+1)p}{q}\right) = e^{-ik_y}(1 - e^{\frac{2i\pi(k+1)p}{q}})e^{ik_y}(1 - e^{-\frac{2i\pi(k+1)p}{q}}) = \alpha_{p/q}(k)\overline{\alpha}_{p/q}(k),$$

where

$$\alpha_{p/q}(k) = e^{-ik_y}(1 - e^{\frac{2i\pi(k+1)p}{q}})$$

and $\overline{\alpha}_{p/q}(k)$ is the complex conjugate. How to derive (9) is explained in Kreft's paper[3] (see the Appendix for details). Note that $a_{p/q}(2j) = 0$ as soon as $q < 2j$.

A closed expression for the quantum Hofstadter trace, which is defined as

$$\mathrm{Tr}\, H^n_{2\pi p/q} = \frac{1}{q}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\sum_{r=1}^{q} E_r^n(k_x,k_y), \tag{10}$$

where one has integrated over the quasi-momenta k_x and $k_y \in [-\pi, \pi]$ the sum of the q eigenenergies $E_r(k_x, k_y)$—the roots of (8)—at a power n, has been obtained[1] in terms of the Kreft coefficients

$$\mathrm{Tr}H^n_{2\pi p/q} = \frac{n}{q}\sum_{k\geq 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-qk}}\frac{\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}\binom{2k}{k}^2 \prod_{j=1}^{\lfloor q/2\rfloor} a_{p/q}(2j)^{\ell_j}, \tag{11}$$

with the generating function

$$\sum_{n\geq 0}\mathrm{Tr}H^n_{2\pi p/q}z^n = \Big(1-\frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\Big)\frac{2}{\pi}K\Big(\frac{16z^{2q}}{b_{p/q}(z)^2}\Big), \tag{12}$$

where K is the complete elliptic integral of the first kind, $\frac{2}{\pi}K(16x) = \sum_{k\geq 0}\binom{2k}{k}^2 x^k$.

III. POINT SPECTRUM TRACE FORMULA AND DENSITY OF STATES

A. Mid-band trace formula

One aims at generalizing (11) and (12) to the almost Mathieu operator case (2). To achieve this goal, first of all, one remarks that the Hofstadter trace (11), valid for all n and q, coincides when $q > n/2$ with the mid-band traces given for the particular cases $n = 2, \ldots, 10$ in Ref. 6. The mid-band trace

$$\mathrm{Tr}_0 H^n_{2\pi p/q} = \frac{1}{q}\sum_{r=1}^{q} E_r^n(0),$$

to be distinguished from the quantum Hofstadter trace (10), is taken solely on the mid-band energies $E_r(0)$, the roots of Ref. 7

$$E^q b_{p/q}(1/E) = 0, \tag{13}$$

to be distinguished from the $E_r(k_x, k_y)$'s, the roots of (8) (for an illustration see Figs. 1 and 2).

It is quite straightforward to obtain for all n and q the mid-band trace formula

$$\mathrm{Tr}_0 H^n_{2\pi p/q} = \frac{n}{q}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2}}\frac{\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}}\prod_{j=1}^{\lfloor q/2\rfloor} a_{p/q}(2j)^{\ell_j}. \tag{14}$$

One can check that the Hofstadter trace (11) and the mid-band trace (14) indeed coincide provided that $q > n/2$ since then the summation index k in (11) necessarily vanishes. A qualitative interpretation for this fact can stem from the classical picture of lattice walks contained in the quantum periodic cell of horizontal length q (the lattice walk the farthest on the horizontal axis from the origin indeed goes to a distance $n/2$).

The mid-band trace (14) has a simple combinatorial interpretation: it is the sum of products of the $a_{p/q}(2j)^{\ell_j}$'s corresponding to partitions of n in even integer parts of size $2j$ [no larger than q since $a_{p/q}(2j) = 0$ as soon as $q < 2j$], i.e., $2\ell_1 + 4\ell_2 + \cdots + 2\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor} = n$, multiplied by the multinomial weight.

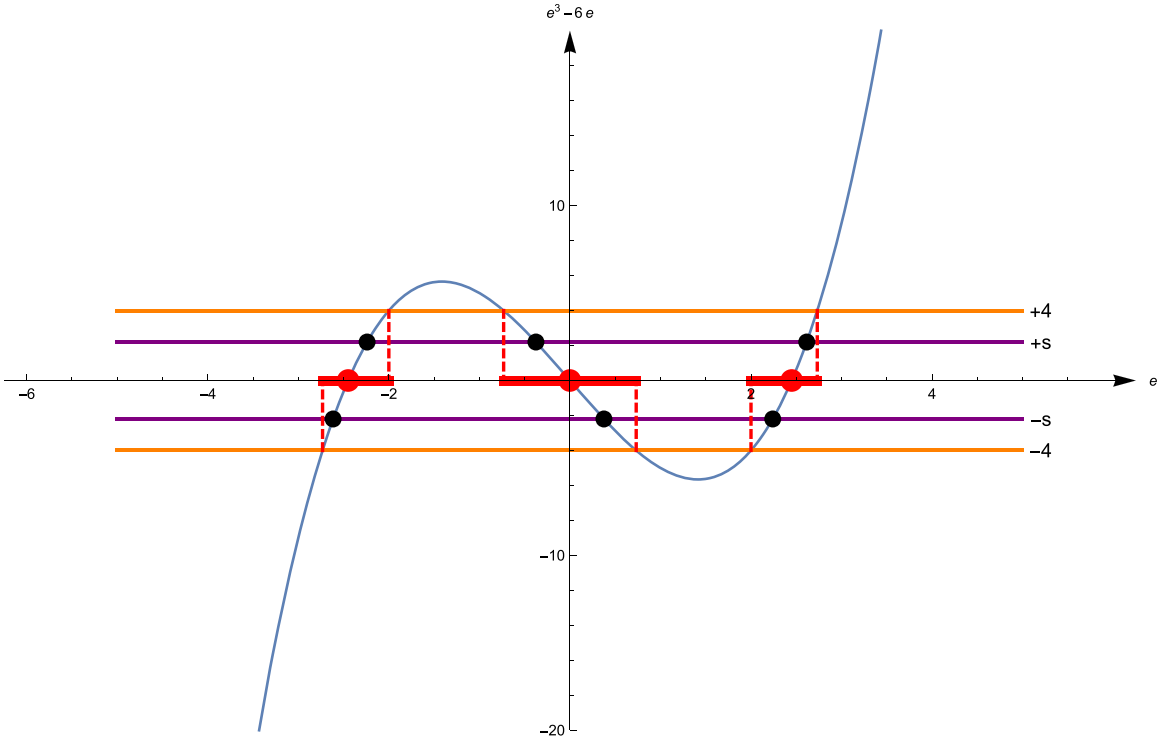

FIG. 1. $p = 1$, $q = 3$: $E^q b_{p/q}(1/E) = E^3 - 6E$; the 3 horizontal red segments are the energy bands; the 3 red dots are the mid-band energies; the 6 black dots are the $\pm s$ energies.

The generating function follows as

$$\sum_{n\geq 0, n \text{ even}} \mathrm{Tr}_0 H^n_{2\pi p/q} z^n = 1 - \frac{z b'_{p/q}(z)}{q b_{p/q}(z)}, \tag{15}$$

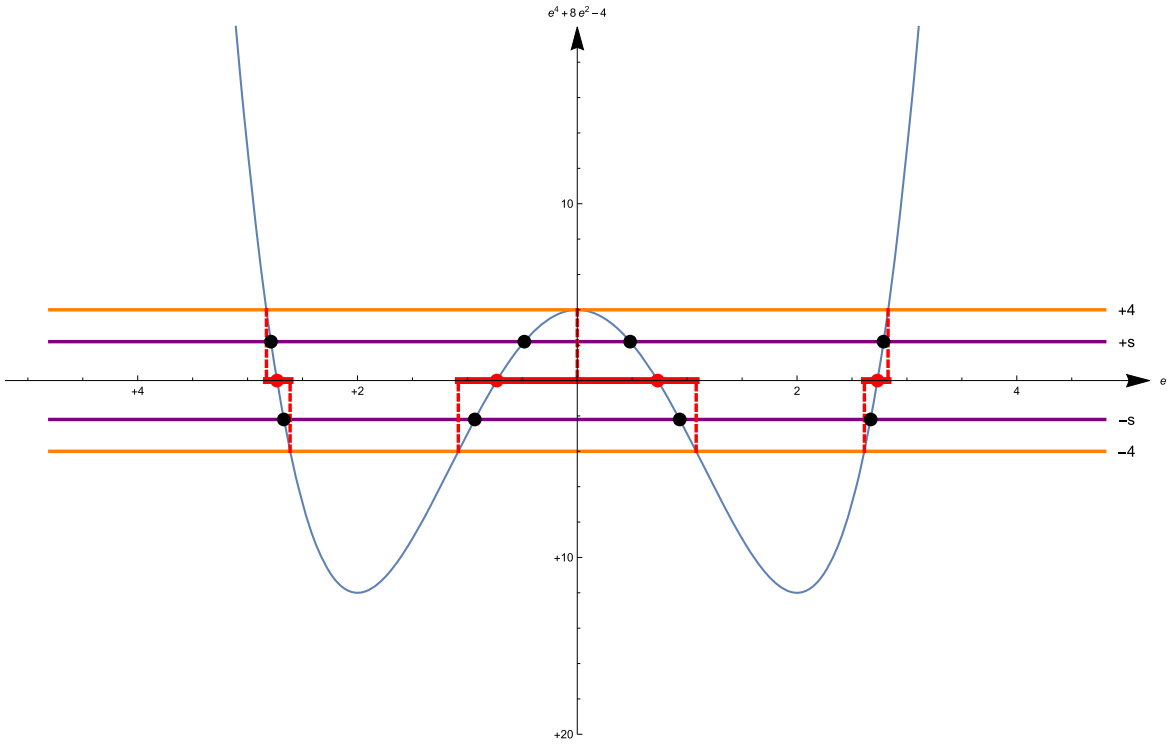

FIG. 2. $p = 1$, $q = 4$: $E^q b_{p/q}(1/E) = E^4 - 8E^2 + 4$; the 4 horizontal red segments are the energy bands; the 4 red dots are the mid-band energies; the 8 black dots are the $\pm s$ energies.

which amounts to nothing else but (13); i.e., the $E_r(0)$'s are the roots of $E^q b_{b/q}(1/E) = 0$. To see this, rewrite

$$\sum_{n\geq 0, n \text{ even}} \mathrm{Tr}_0 H^n_{2\pi p/q} z^n = \sum_{n\geq 0, n \text{ even}} \frac{1}{q}\Big(\sum_{r=1}^{q} E_r^n(0)\Big) z^n = \frac{1}{q}\sum_{r=1}^{q} \sum_{n\geq 0, n \text{ even}} (zE_r(0))^n$$
$$= \frac{1}{q}\sum_{r=1}^{q} \frac{1}{1-z^2E_r^2(0)} = \frac{1}{2q}\sum_{r=1}^{q}\Big(\frac{1}{1-zE_r(0)} + \frac{1}{1+zE_r(0)}\Big) = \frac{1}{q}\sum_{r=1}^{q}\frac{1}{1-zE_r(0)}$$

so that (15) becomes

$$\frac{1}{q}\sum_{r=1}^{q}\frac{1}{1-zE_r(0)} = 1 - \frac{zb'_{p/q}(z)}{qb_{p/q}(z)}. \tag{16}$$

On the other hand, (13) rewrites as

$$(1/z)^q b_{p/q}(z) = \prod_{r=1}^{q}(1/z - E_r(0)),$$

that is,

$$b_{p/q}(z) = \prod_{r=1}^{q}(1 - zE_r(0))$$

so that

$$(\log(b_{p/q}(z)))' = \sum_{r=1}^{q}\frac{-E_r(0)}{1-zE_r(0)} = \frac{1}{z}\sum_{r=1}^{q}\Big(1 - \frac{1}{1-zE_r(0)}\Big)$$

or

$$\frac{b_{p/q}(z)'}{b_{p/q}(z)} = \frac{1}{z}\Big(q - \sum_{r=1}^{q}\frac{1}{1-zE_r(0)}\Big),$$

which is (16).

B. $\pm s$ trace formula

More generally, one can consider the $\pm s$ spectrum traces

$$\mathrm{Tr}_{\pm s} H^n_{2\pi p/q} = \frac{1}{2q}\Big(\sum_{r=1}^{q} E_r^n(s) + \sum_{r=1}^{q} E_r^n(-s)\Big)$$

taken on the $2q$ roots $E_r(s)$ and $E_r(-s)$ of

$$E^q b_{p/q}(1/E) = s \text{ and } E^q b_{p/q}(1/E) = -s \tag{17}$$

with $-4 \leq s \leq 4$ since $-4 \leq 2(\cos(qk_x) + \cos(qk_y)) \leq 4$ in (8). The mid-band spectrum is obtained for $s = 0$, and the edge-band spectrum is obtained for $s = 4$, which is of particular interest as well (see Figs. 1 and 2).

Following the same line of reasoning as for the mid-band spectrum, one obtains the $\pm s$ spectrum trace generating function

$$\sum_{n\geq 0, n \text{ even}} \mathrm{Tr}_{\pm s} H^n_{2\pi p/q} z^n = 1 - \frac{z(b_{p/q}(z) - sz^q)'}{2q(b_{p/q}(z) - sz^q)} - \frac{z(b_{p/q}(z) + sz^q)'}{2q(b_{p/q}(z) + sz^q)}$$
$$= 1 - \frac{z(b^2_{p/q}(z) - s^2z^{2q})'}{2q(b^2_{p/q}(z) - s^2z^{2q})}$$
$$= \Big(1 - \frac{zb'_{p/q}(z)}{qb_{p/q}(z)}\Big)\frac{1}{1 - s^2(\frac{z^q}{b_{p/q}(z)})^2}, \tag{18}$$

which rightly reduces to the mid-band case (15) when $s = 0$. Again (18) is a mere rewriting of the $E_r(s)$'s and $E_r(-s)$'s being the roots of $E^q b_{p/q}(1/E) = \pm s$ in (17).

One has likewise the $\pm s$ trace formula

$$\mathrm{Tr}_{\pm s} H^n_{2\pi p/q} = \frac{n}{q} \sum_{k\geq 0} \sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0 \\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor \ell_{\lfloor q/2\rfloor}=n/2-qk}} \frac{\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k} s^{2k} \prod_{j=1}^{\lfloor q/2\rfloor} a_{p/q}(2j)^{\ell_j}, \tag{19}$$

which again reduces to the mid-band trace (14) when $s = 0$. The combinatorial interpretation of (19) is again simple in terms of products of s^2 and of the $a_{p/q}(2j)$'s corresponding to all partitions of n in even integer parts of size $2q$ and $2j$, respectively.

Again, as soon as $q > n/2$, the trace $\mathrm{Tr}_{\pm s} H^n_{2\pi p/q}$ in (19) does not depend on s anymore and coincides with the Hofstadter trace (11) and, by the same token, with the mid-band trace (14).

C. Density of states

One remarks next that the Hofstadter quantum trace $\mathrm{Tr} H^n_{2\pi p/q}$ in (11) can be recovered from the $\pm s$ spectrum trace $\mathrm{Tr}_{\pm s} H^n_{2\pi p/q}$ in (19) if one replaces s^{2k} by $\binom{2k}{k}^2$. This replacement amounts to an integration of (19) over $s \in [-4, 4]$ with the density of state $\rho(s)$,

$$\int_{-4}^{4} \mathrm{Tr}_{\pm s} H^n_{2\pi p/q} \rho(s) ds = \mathrm{Tr} H^n_{2\pi p/q} \tag{20}$$

such that

$$\int_{-4}^{4} s^{2k} \rho(s) ds = \binom{2k}{k}^2. \tag{21}$$

Clearly the free density of states on the 2d lattice,

$$\rho(s) = 1/(2\pi^2) K(1 - s^2/16), \tag{22}$$

enforces (21): it is the density of states for the spectrum $s = 2(\cos(qk_x) + \cos(qk_y))$. Again, as soon as $q > n/2$, the integration in (20) becomes trivial, i.e., the identity. Note that in the spirit of Ref. 8, one can make the change of variable $s = \pm E^q b_{p/q}(1/E)$ in (21) to obtain

$$\int_{-4}^{4} (E^q b_{p/q}(1/E))^{2k} \rho_{p/q}(E) dE = \binom{2k}{k}^2,$$

where $\rho_{p/q}(E)$ is the Hofstadter density of states. This yields the trace sum rule

$$\mathrm{Tr}(H^q_{2\pi p/q} b_{p/q}(1/H_{2\pi p/q}))^{2k} = \binom{2k}{k}^2$$

or

$$\mathrm{Tr}\Big(\sum_{j=0}^{[\frac{q}{2}]} a_{p/q}(2j) H^{q-2j}_{2\pi p/q}\Big)^{2k} = \binom{2k}{k}^2,$$

which is an inversion of (11).

For the generating function as well, which is given by

$$\int_{-4}^{4} \sum_n \mathrm{Tr}_{\pm s} H^n_{2\pi p/q} z^n \rho(s) ds = \sum_n \mathrm{Tr} H^n_{2\pi p/q} z^n,$$

one uses (12), (18), and (22) so that

$$\int_{-4}^{4} \Big(1 - \frac{z(b^2_{p/q}(z) - s^2 z^{2q})'}{2q(b^2_{p/q}(z) - s^2 z^{2q})}\Big) \frac{1}{2\pi^2} K\Big(1 - \frac{s^2}{16}\Big) ds = \Big(1 - \frac{z b'_{p/q}(z)}{q b_{p/q}(z)}\Big) \frac{2}{\pi} K\Big(16\Big(\frac{z^q}{b_{p/q}(z)}\Big)^2\Big)$$

has to be satisfied. After simplification, this narrows down to

$$\int_{-4}^{4} \frac{1}{2\pi^2} K\left(1-\frac{s^2}{16}\right) \frac{1}{1-s^2(\frac{z^q}{b_{p/q}(z)})^2} ds = \frac{2}{\pi} K\Big(16\Big(\frac{z^q}{b_{p/q}(z)}\Big)^2\Big),$$

i.e.,

$$\int_{-4}^{4} K\left(1-\frac{s^2}{16}\right) \frac{1}{1-s^2 z^2} ds = 4\pi K(16z^2),$$

which is nothing but the complete elliptic integral of the first kind being the generating function for the square of the binomial coefficients, i.e., $\frac{2}{\pi} K(16z^2) = \sum_k \binom{2k}{k}^2 z^{2k}$.

IV. $\lambda \neq 2$: POINT SPECTRUM TRACE FORMULA AND DENSITY OF STATES

All these considerations can be extended when $\lambda \neq 2$ to the almost Mathieu case (2) whose secular matrix is

$$m^{(\lambda)}_{p/q}(E,k_x,k_y) = \begin{pmatrix} \lambda\cos(k_y) - E & 1 & 0 & \cdots & 0 & e^{-iqk_x} \\ 1 & \lambda\cos(k_y + \frac{2\pi p}{q}) - E & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ e^{iqk_x} & 0 & 0 & \cdots & 1 & \lambda\cos(k_y + (q-1)\frac{2\pi p}{q}) - E \end{pmatrix}. \tag{23}$$

Thanks to the identity

$$\det(m^{(\lambda)}_{p/q}(E,k_x,k_y)) = \det(m^{(\lambda)}_{p/q}(E,0,0)) - 2(-1)^q(\cos(qk_x) - 1 + (\lambda/2)^q(\cos(qk_y) - 1)),$$

the Schrödinger equation becomes

$$\det(m^{(\lambda)}_{p/q}(E,0,0)) = 2(-1)^q(\cos(qk_x) - 1 + (\lambda/2)^q(\cos(qk_y) - 1)). \tag{24}$$

Again one introduces the polynomial $b^{(\lambda)}_{p/q}(z)$ and its coefficients $-a^{(\lambda)}_{p/q}(2j)$ [with $a^{(\lambda)}_{p/q}(0) = -1$],

$$b^{(\lambda)}_{p/q}(z) = -\sum_{j=0}^{[\frac{q}{2}]} a^{(\lambda)}_{p/q}(2j) z^{2j} \tag{25}$$

such that $\det(m^{(\lambda)}_{p/q}(E,0,0))$ rewrites as

$$\det(m^{(\lambda)}_{p/q}(E,0,0)) + 2(-1)^q(1 + (\lambda/2)^q) = (-1)^q E^q b^{(\lambda)}_{p/q}(1/E) \tag{26}$$

so that (24) becomes

$$E^q b^{(\lambda)}_{p/q}(1/E) = 2(\cos(qk_x) + (\lambda/2)^q \cos(qk_y)). \tag{27}$$

In the Appendix, we show how to get a closed expression for the generalized Kreft coefficients $a^{(\lambda)}_{p/q}(2i)$'s in (25) following the steps of Ref. 3. This procedure coalesces to

$$a^{(\lambda)}_{p/q}(2j) = (-1)^{j+1} \sum_{k_1=0}^{q-2j} \sum_{k_2=0}^{k_1} \cdots \sum_{k_j=0}^{k_{j-1}} \alpha^{(\lambda)}_{p/q}(k_1+2j-2)\overline{\alpha}^{(\lambda)}_{p/q}(k_1+2j-2)$$
$$\alpha^{(\lambda)}_{p/q}(k_2+2j-4)\overline{\alpha}^{(\lambda)}_{p/q}(k_2+2j-4)\ldots\alpha^{(\lambda)}_{p/q}(k_j)\overline{\alpha}^{(\lambda)}_{p/q}(k_j) \tag{28}$$

with building blocks

$$\alpha^{(\lambda)}_{p/q}(k)\overline{\alpha}^{(\lambda)}_{p/q}(k),$$

where

$$\alpha^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{-ik_y}\left(1 - e^{\frac{2i\pi(k+1)p}{q}}\right)$$

and

$$\overline{\alpha}^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{ik_y}\left(1 - (2/\lambda)^2 e^{-\frac{2i\pi(k+1)p}{q}}\right).$$

When $\lambda \neq 2$, even though $\overline{\alpha}^{(\lambda)}_{p/q}(k)$ is not anymore the complex conjugate of $\alpha^{(\lambda)}_{p/q}(k)$, it is still true that $a^{(\lambda)}_{p/q}(2j)$ in (28) is real. Indeed its imaginary part cancels because of

$$\sum_{k=1}^{q} \mathrm{e}^{\frac{2i\pi kp}{q}j} = 0$$

when $q > j$, being a sum of jth powers of qth roots of unity. For example, when $j = 1$,

$$\begin{aligned} a^{(\lambda)}_{p/q}(2) = \sum_{k=0}^{q-2} \alpha^{(\lambda)}_{p/q}(k)\overline{\alpha}^{(\lambda)}_{p/q}(k) &= (\lambda/2)^2 \sum_{k=0}^{q-2}\left(1 - e^{\frac{2i\pi(k+1)p}{q}} + (2/\lambda)^2 - (2/\lambda)^2 e^{-\frac{2i\pi(k+1)p}{q}}\right) \\ &= (\lambda/2)^2 \sum_{k=0}^{q-1}\left(1 - e^{\frac{2i\pi(k+1)p}{q}} + (2/\lambda)^2 - (2/\lambda)^2 e^{-\frac{2i\pi(k+1)p}{q}}\right) \\ &= (\lambda/2)^2 \sum_{k=0}^{q-1}\left(1 + (2/\lambda)^2\right) = q\left(1 + (\lambda/2)^2\right). \end{aligned}$$

Of all that precedes, in the $\lambda \neq 2$ almost Mathieu case, the $\pm s$ spectrum traces and their generating function are directly obtained by replacing in the Hofstadter $\pm s$ spectrum traces and generating functions (19) and (18) the $a_{p/q}(2j)$'s by the $a^{(\lambda)}_{p/q}(2j)$'s and so the polynomial $b_{p/q}(z)$ by $b^{(\lambda)}_{p/q}(z)$. This is due to the purely algebraic construction of these traces in terms of the $a_{p/q}(2j)$'s via the roots of (17) and therefore, in the $\lambda \neq 2$ case, the roots of

$$E^q b^{(\lambda)}_{p/q}(1/E) = \pm s$$

with $0 \leq |s| \leq 2(1 + (\lambda/2)^q)$, since from (27) necessarily $0 \leq |2(\cos(qk_x) + (\lambda/2)^q \cos(qk_y))| \leq 2(1 + (\lambda/2)^q)$.

As stated in the Introduction, one wishes to obtain a closed formula for the almost Mathieu quantum trace defined as

$$\mathrm{Tr}\,(H^{(\lambda)}_{2\pi p/q})^n = \frac{1}{q}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\sum_{r=1}^{q}(E^{(\lambda)}_r(k_x, k_y))^n, \tag{29}$$

where the $E^{(\lambda)}_r(k_x, k_y)$'s are the roots of (27). To do so, as in the Hofstadter case, one aims at integrating over $s \in [-2(1 + (\lambda/2)^q), 2(1 + (\lambda/2)^q)]$ the $\pm s$ spectrum trace with the density of state $\rho^{(\lambda)}(s)$,

$$\int_{-2(1+(\lambda/2)^q)}^{2(1+(\lambda/2)^q)} \mathrm{Tr}_s(H^{(\lambda)}_{2\pi p/q})^n \rho^{(\lambda)}(s)ds = \mathrm{Tr}(H^{(\lambda)}_{2\pi p/q})^n,$$

which is such that

$$\int_{-2(1+(\lambda/2)^q)}^{2(1+(\lambda/2)^q)} s^{2k}\rho^{(\lambda)}(s)ds = \binom{2k}{k}\sum_{k_1=0}^{k}\binom{k}{k_1}^2(\lambda/2)^{2qk_1} \tag{30}$$

in analogy to (21). A derivation of $\rho^{(\lambda)}(s)$ enforcing (30) is given in the Appendix. This density of states is the λ-deformation of $\rho(s)$ in (22) for the 2d lattice spectrum $s = 2(\cos(qk_x) + (\lambda/2)^q \cos(qk_y))$.

Putting all the steps above together, namely, in (19) replacing both the $a_{p/q}(2j)$'s by the $a^{(\lambda)}_{p/q}(2j)$'s and s^{2k} by $\binom{2k}{k}\sum_{k_1=0}^{k}\binom{k}{k_1}^2(\lambda/2)^{2qk_1}$, the almost Mathieu operator quantum trace (29) ends up as

$$\mathrm{Tr}\,(H^{(\lambda)}_{2\pi p/q})^n = \frac{n}{q}\sum_{k\geq 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-qk}} \frac{\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}\binom{2k}{k}\sum_{k_1=0}^{k}\binom{k}{k_1}^2(\lambda/2)^{2qk_1}$$
$$\prod_{j=1}^{\lfloor q/2\rfloor} a^{(\lambda)}_{p/q}(2j)^{\ell_j}, \tag{31}$$

which is a λ-deformation of the quantum Hofstadter trace (11).

One also gets the generating function that generalizes (12),

$$\sum_{n\geq 0} Z^{(\lambda)}_n(e^{2i\pi p/q})z^n = \Big(1-\frac{z(b^{(\lambda)}_{p/q}(z))'}{qb^{(\lambda)}_{p/q}(z)}\Big)\sum_{k\geq 0}\binom{2k}{k}\sum_{k_1=0}^{k}\binom{k}{k_1}^2(\lambda/2)^{2qk_1}\Big(\frac{z^q}{b^{(\lambda)}_{p/q}(z)}\Big)^{2k}, \tag{32}$$

where $\sum_{k\geq 0}\binom{2k}{k}\sum_{k_1=0}^{k}\binom{k}{k_1}^2(\lambda/2)^{2qk_1}x^k$ can be viewed again in terms of the complete elliptic integral $(2/\pi)K(16x)=\sum_{k\geq 0}\binom{2k}{k}^2x^k$. Indeed thanks to the identity

$$\sum_{k=0}^{\infty}\binom{2k}{k}x^k\sum_{k_1=0}^{k}\binom{k}{k_1}^2y^{2k_1} = \frac{1}{\sqrt{1-4x(1-y)^2}}\sum_{k=0}^{\infty}\binom{2k}{k}^2\Big(\frac{xy}{1-4x(1-y)^2}\Big)^k, \tag{33}$$

(32) can be summed up to

$$\sum_{n\geq 0} Z^{(\lambda)}_n(e^{2i\pi p/q})z^n = \Big(1-\frac{z(b^{(\lambda)}_{p/q}(z))'}{qb^{(\lambda)}_{p/q}(z)}\Big)\frac{1}{\sqrt{1-4(\frac{z^q}{b^{(\lambda)}_{p/q}(z)})^2(1-(\lambda/2)^q)^2}}$$
$$\times\frac{2}{\pi}K\Big(\frac{16z^{2q}(\lambda/2)^q}{b^{(\lambda)}_{p/q}(z)^2-4z^{2q}(1-(\lambda/2)^q)^2}\Big) \tag{34}$$

which rightly reduces to (12) when $\lambda=2$ [see Subsection 2 in the Appendix for a derivation of the density of state $\rho^{(\lambda)}(s)$ again in terms of the complete elliptic integral]. One can also check that the expression (34) for the generating function can be retrieved by starting from (29) and integrating with respect to the momenta k_x and k_y.

To see why (33) holds, first note that $\sum_{k_1=0}^{k}\binom{k}{k_1}^2y^{2k_1}$ is the coefficient of t^0 in

$$\Big(1+\frac{y}{t}\Big)^k(1+yt)^k = \sum_{i=0}^{k}\binom{k}{i}y^it^{-i}\sum_{j=0}^{k}\binom{k}{j}y^jt^j.$$

Thus the left-hand side of (33) is the coefficient of t^0 in

$$\sum_{k=0}^{\infty}\binom{2k}{k}x^k\Big(1+\frac{y}{t}\Big)^k(1+yt)^k = \frac{1}{\sqrt{1-4x(1+y/t)(1+yt)}}$$
$$= \frac{1}{\sqrt{1-4x(1-y)^2-4xy(1+t)^2/t}}$$
$$= \frac{1}{\sqrt{1-4x(1-y)^2}}\cdot\frac{1}{\sqrt{1-4\frac{xy}{1-4x(1-y)^2}\cdot\frac{(1+t)^2}{t}}}$$
$$= \frac{1}{\sqrt{1-4x(1-y)^2}}\cdot\sum_{k=0}^{\infty}\binom{2k}{k}\Big(\frac{xy}{1-4x(1-y)^2}\Big)^k\Big(\frac{(1+t)^2}{t}\Big)^k.$$

Now it only remains to see that the coefficient of t^0 in $(\frac{(1+t)^2}{t})^k$ is precisely $\binom{2k}{k}$.

Note finally that one can check that the Aubry duality,[9]

$$\mathrm{Tr}\,(H^{(\lambda)}_{2\pi p/q})^n = (\frac{\lambda}{2})^n \mathrm{Tr}\,(H^{(4/\lambda)}_{2\pi p/q})^n, \tag{35}$$

holds, as it should. This happens because the generalized Kreft coefficients (28) themselves obey the duality

$$a^{(\lambda)}_{p/q}(2j) = (\frac{\lambda}{2})^{2j}\, a^{(4/\lambda)}_{p/q}(2j) \Rightarrow b^{(\lambda)}_{p/q}(z) = b^{(4/\lambda)}_{p/q}(\frac{\lambda z}{2}) \tag{36}$$

which follows from

$$\mathrm{Re}\Big(\alpha^{(\lambda)}_{p/q}(k)\overline{\alpha}^{(\lambda)}_{p/q}(k)\Big) = \Big(\frac{\lambda}{2}\Big)^2 \mathrm{Re}\Big(\alpha^{(4/\lambda)}_{p/q}(k)\overline{\alpha}^{(4/\lambda)}_{p/q}(k)\Big)$$

[only the real part is needed here since $a^{(\lambda)}_{p/q}(2j)$ is real]. The duality (35) then follows from (31) and the duality (36),

$$\mathrm{Tr}\,(H^{(\lambda)}_{2\pi p/q})^n = \frac{n}{q}\sum_{k\geq 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-qk}} \frac{\binom{2k}{k}\sum_{k_1=0}^k \binom{k}{k_1}^2 (\lambda/2)^{2qk_1}\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}$$

$$(\lambda/2)^{\sum_{j=1}^{\lfloor q/2\rfloor} 2j\ell_j}\prod_{j=1}^{\lfloor q/2\rfloor} a^{(4/\lambda)}_{p/q}(2j)^{\ell_j}$$

$$= \frac{n}{q}\sum_{k\geq 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-qk}} \frac{\binom{2k}{k}\sum_{k_1=0}^k \binom{k}{k_1}^2 (\lambda/2)^{2qk_1}\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}$$

$$(\lambda/2)^{n-2qk}\prod_{j=1}^{\lfloor q/2\rfloor} a^{(4/\lambda)}_{p/q}(2j)^{\ell_j}$$

$$= (\lambda/2)^n \frac{n}{q}\sum_{k\geq 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-qk}} \frac{\binom{2k}{k}\sum_{k_1=0}^k \binom{k}{k_1}^2 (2/\lambda)^{2qk-2qk_1}\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}$$

$$\prod_{j=1}^{\lfloor q/2\rfloor} a^{(4/\lambda)}_{p/q}(2j)^{\ell_j}$$

$$\overset{k_1'=k-k_1}{=} (\lambda/2)^n \frac{n}{q}\sum_{k\geq 0}\sum_{\substack{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor}\geq 0\\ \ell_1+2\ell_2+\cdots+\lfloor q/2\rfloor\ell_{\lfloor q/2\rfloor}=n/2-qk}} \frac{\binom{2k}{k}\sum_{k_1'=0}^k \binom{k}{k_1'}^2 (2/\lambda)^{2qk_1'}\binom{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}{\ell_1,\ell_2,\ldots,\ell_{\lfloor q/2\rfloor},2k}}{\ell_1+\ell_2+\cdots+\ell_{\lfloor q/2\rfloor}+2k}$$

$$\prod_{j=1}^{\lfloor q/2\rfloor} a^{(4/\lambda)}_{p/q}(2j)^{\ell_j} = (\lambda/2)^n \mathrm{Tr}\,(H^{(4/\lambda)}_{2\pi p/q})^n.$$

V. CONCLUSION

One has obtained the λ-deformation of the quantum trace (11) in the form of (31). Both trace formulae have a similar structure, with clearly (31), the almost Mathieu case, reducing when $\lambda = 2$ to (11), the Hofstadter case. Going back for a moment to random walks on a lattice, it would certainly be interesting to look at possible interpretations of (31) in the context of asymmetric paths with unequal probabilities on the horizontal and vertical axis.

On the other hand, our results are directly relevant for problems related to Calabi-Yau geometry. A recent work[10] indicates that there exists in the rational case a relation between the almost Mathieu

operator and the relativistic Toda lattice. As pointed out in Sec. 2 of Ref. 10, there is an invariance under the modular double operation exchanging $\gamma = 2\pi p/q$ and $\tilde{\gamma} = 2\pi q/p$ (respectively, $\hbar$ and $\tilde{\hbar}$ in the notations of Ref. 10) of the relativistic relative 2-body Toda Hamiltonian

$$H = \lambda(e^{p} + e^{-p}) + e^{x} + e^{-x}, \quad [x, p] = i\gamma, \tag{37}$$

where, in Ref. 10, λ is denoted as R^2. The eigenvalues E and $\tilde{E}$ corresponding to γ and $\tilde{\gamma}$ satisfy the polynomial identity $P_{p/q}(E) = P_{q/p}(\tilde{E})$, where $P_{p/q}(E)$ is a polynomial of degree q [see (2.19) in Ref. 10]. Now this polynomial is identical to the polynomial $E^q b^{(\lambda)}_{p/q}(1/E)$ introduced in (25) and (26) which encodes the $\{k_x, k_y\}$-independent part of the determinant of the almost Mathieu Schrödinger equation encapsulated in $m^{(\lambda)}_{p/q}(E, k_x, k_y)$. In the present work, we have precisely obtained in (28) a closed expression for these polynomials in terms of the generalized Kreft coefficients.

It would certainly be rewarding to see if (28) can bring any pertinent information related to the various questions raised in Ref. 10, in particular, regarding the quantum A-period for the modulus of the underlying Calabi-Yau geometry. Finally, in the context of the Hofstadter model itself, the true role of the double modular transformation $\gamma \to \tilde{\gamma}$ remains to be elucidated.

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APPENDIX A: KREFT'S COEFFICIENTS CONSTRUCTION

Following Kreft,[3] we show how to get a closed expression for the polynomial (26), i.e., for the Kreft coefficients $a^{(\lambda)}_{p/q}(2j)$ in $b^{(\lambda)}_{p/q}(z) = -\sum_{j=0}^{[\frac{q}{2}]} a^{(\lambda)}_{p/q}(2j) z^{2j}$ as defined in (25).

1. $\lambda = 2$

One aims at transforming the matrix $m_{p/q}\Big(E, k_x, k_y\Big)$ in (3) into a tridiagonal one by an appropriate change of basis. First, let us do the change of basis

$$m_1 = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & e^{ik_x} & 0 & \cdots & 0 & 0 \\ 0 & 0 & e^{i2k_x} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & e^{i(q-2)k_x} & 0 \\ 0 & 0 & 0 & \cdots & 0 & e^{i(q-1)k_x} \end{pmatrix}$$

so that $m_{p/q}\Big(E, k_x, k_y\Big)$ rewrites as

$$m_1^{-1} m_{p/q}\Big(E, k_x, k_y\Big) m_1 = \begin{pmatrix} 2\cos(k_y) - E & e^{ik_x} & 0 & \cdots & 0 & e^{-ik_x} \\ e^{-ik_x} & 2\cos(k_y + \frac{2\pi p}{q}) - E & e^{ik_x} & \cdots & 0 & 0 \\ 0 & e^{-ik_x} & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & e^{ik_x} \\ e^{ik_x} & 0 & 0 & \cdots & e^{-ik_x} & 2\cos(k_y + (q-1)\frac{2\pi p}{q}) - E \end{pmatrix}.$$

In this new basis, the Schrödinger equation (1) with $\Phi_{m+q} = e^{iqk_x}\Phi_m$ becomes

$$e^{ik_x}\Phi'_{m+1} + e^{-ik_x}\Phi'_{m-1} + 2\cos\Big(k_y + \gamma m\Big)\Phi'_m = E\Phi'_m, \quad \Phi'_{m+q} = \Phi'_m.$$

Then let us do a second change of basis m_2 with matrix element

$$m_{jk} = \frac{1}{\sqrt{q}}(-1)^{pk} e^{\frac{2i\pi p}{q}(jk-k^2/2)}, \quad k,j \in \{0,1,\dots,q-1\}.$$

Putting together m_1 and m_2 amounts to the change of basis $m_1 m_2$ with matrix element $e^{ikk_x} m_{jk} = e^{ikk_x} \frac{1}{\sqrt{q}}(-1)^{pk} e^{\frac{2i\pi p}{q}(jk-k^2/2)}$,

$$(m_1 m_2)^{-1} m_{p/q}\big(E,k_x,k_y\big) m_1 m_2 = \begin{pmatrix} -E & \alpha_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}_{p/q}(q-1) \\ \overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-2) \\ \alpha_{p/q}(q-1) & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-2) & -E \end{pmatrix}, \tag{A1}$$

where $\alpha_{p/q}(k) = e^{-ik_y} - (-1)^{(p+1)} e^{\frac{2i\pi p}{q}(k+1/2)+ik_x}$ and $\overline{\alpha}_{p/q}(k)$ is its complex conjugate and accordingly

$$\alpha_{p/q}(m)\tilde{\Phi}_{m+1} + \overline{\alpha}_{p/q}(m-1)\tilde{\Phi}_{m-1} = E\tilde{\Phi}_m, \quad \tilde{\Phi}_{m+q} = \tilde{\Phi}_m. \tag{A2}$$

Both corners $\alpha_{p/q}(q-1)$ and $\overline{\alpha}_{p/q}(q-1)$ in the matrix (A1) can be canceled if $e^{i(k_x+k_y)} = (-1)^{(p+1)} e^{-\frac{2i\pi p}{q}(q-1+1/2)} = (-1)^{(p+1)} e^{\frac{i\pi p}{q}}$, i.e., if $k_x + k_y = \pi(p+1) + \frac{\pi p}{q}$. The matrix is then tridiagonal with a determinant in (4) equal to $(-1)^q E^q b_{p/q}(1/E)$, since the trigonometric part vanishes as well; indeed

$$\begin{aligned} \cos(qk_x) + \cos(qk_y) &= 2\cos\Big(\frac{q(k_x+k_y)}{2}\Big)\cos\Big(\frac{q(k_x-k_y)}{2}\Big) \\ &= 2\cos\Big(\frac{\pi(p+q(p+1))}{2}\Big)\cos\Big(\frac{q(k_x-k_y)}{2}\Big) \\ &= 0 \end{aligned}$$

due to $p + q(p+1)$ being always odd since p and q are co-prime.

One gets the tridiagonal matrix

$$\begin{pmatrix} -E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0 \\ \overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-2) \\ 0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-2) & -E \end{pmatrix}, \tag{A3}$$

where $\alpha_{p/q}(k)$, using $e^{i(k_x+k_y)} = (-1)^{(p+1)} e^{\frac{i\pi p}{q}}$, has simplified to $\alpha_{p/q}(k) = e^{-ik_y}(1 - e^{\frac{2i\pi(k+1)p}{q}})$. The matrix (A3) does not depend anymore on k_x nor on k_y and its determinant satisfies a recursion (see Ref. 3) leading, respectively, to the Kreft polynomial and Kreft coefficients (7) and (9).

2. $\lambda \neq 2$

One uses the same method as above to find a closed expression for the polynomial $b^{(\lambda)}_{p/q}(1/E)$, namely, transform the matrix $m^{(\lambda)}_{p/q}\left(E, k_x, k_y\right)$ in (23) into a tridiagonal one. To do so, use the same change of basis $m_1 m_2$ as above so that

$$
\begin{aligned}
&(m_1 m_2)^{-1} m^{(\lambda)}_{p/q}\left(E, k_x, k_y, \right) m_1 m_2 \\
&= \begin{pmatrix}
-E & \alpha^{(\lambda)}_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}^{(\lambda)}_{p/q}(q-1) \\
\overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\
\alpha^{(\lambda)}_{p/q}(q-1) & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E
\end{pmatrix}
\end{aligned}
\tag{A4}
$$

with $\alpha^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{-ik_y} - (-1)^{p+1} e^{i\frac{2\pi p}{q}(k+1/2)+ik_x}$ and $\overline{\alpha}^{(\lambda)}_{p/q}(k)$ its complex conjugate. Moreover, we have a resulting Schrödinger equation identical to (A2) provided that $\alpha_{p/q}(k)$ is replaced with $\alpha^{(\lambda)}_{p/q}(k)$.

Contrary to the Hofstadter case $\lambda = 2$, both corners $\alpha^{(\lambda)}_{p/q}(q-1)$ and $\overline{\alpha}^{(\lambda)}_{p/q}(q-1)$ in the matrix (A4) cannot simultaneously vanish. One can still choose to have the lower left corner $\alpha^{(\lambda)}_{p/q}(q-1)$ to vanish: this amounts to $e^{i(k_x+k_y)} = (-1)^{p+1}(\lambda/2)e^{-i\frac{2\pi p}{q}(q-1+1/2)} = (-1)^{p+1}(\lambda/2)e^{\frac{i\pi p}{q}}$, which can only be achieved for a complex $k_x + k_y$ [namely, $k_x + k_y = -i\log(\lambda/2) + \frac{\pi p}{q} + \pi(p+1)$] so that $e^{-i(k_x+k_y)} = (-1)^{p+1}(2/\lambda)e^{-\frac{i\pi p}{q}}$. The matrix (A4) then becomes

$$
\begin{pmatrix}
-E & \alpha^{(\lambda)}_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}^{(\lambda)}_{p/q}(q-1) \\
\overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\
0 & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E
\end{pmatrix},
\tag{A5}
$$

where $\alpha^{(\lambda)}_{p/q}(k)$ and $\overline{\alpha}^{(\lambda)}_{p/q}(k)$ have simplified to $\alpha^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{-ik_y}(1 - e^{\frac{2i\pi(k+1)p}{q}})$ and $\overline{\alpha}^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{ik_y}(1 - (2/\lambda)^2 e^{-\frac{2i\pi(k+1)p}{q}})$. Note that $\overline{\alpha}^{(\lambda)}_{p/q}(k)$ is not anymore the complex conjugate of $\alpha^{(\lambda)}_{p/q}(k)$.

By expanding the determinant of (A5) with respect to the elements of the first row

$$
\begin{vmatrix}
-E & \alpha^{(\lambda)}_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}^{(\lambda)}_{p/q}(q-1) \\
\overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\
0 & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E
\end{vmatrix}
= -E
\begin{vmatrix}
-E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\
\overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\
0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E
\end{vmatrix}
$$

$$
- \alpha^{(\lambda)}_{p/q}(0)\overline{\alpha}^{(\lambda)}_{p/q}(0)
\begin{vmatrix}
-E & \alpha^{(\lambda)}_{p/q}(2) & \cdots & 0 & 0 \\
\overline{\alpha}^{(\lambda)}_{p/q}(2) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\
0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E
\end{vmatrix}
$$

$$
+ (-1)^{q+1}\overline{\alpha}^{(\lambda)}_{p/q}(q-1)
\begin{vmatrix}
\overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-3) & -E \\
0 & 0 & 0 & \cdots & 0 & \overline{\alpha}^{(\lambda)}_{p/q}(q-2)
\end{vmatrix}, \tag{A6}
$$

it is immediate to see that the part that depends on k_x or k_y can only come from the last term of (A6), i.e., from the upper right corner $\overline{\alpha}^{(\lambda)}_{p/q}(q-1)$. Therefore to get the desired k_x, k_y-independent polynomial $E^q b^{(\lambda)}_{p/q}(1/E)$, all that is needed is the determinant of the tridiagonal matrix

$$
\begin{pmatrix}
-E & \alpha^{(\lambda)}_{p/q}(0) & 0 & \cdots & 0 & 0 \\
\overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\
0 & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E
\end{pmatrix}
$$

which finally yields the $\lambda \neq 2$ Kreft polynomial and Kreft coefficients (26) and (28).

APPENDIX B: DENSITY OF STATES $\rho^{(\lambda)}(s)$

To simplify the notations, let us denote in this section $(\lambda/2)^q$ by $\tilde{\lambda}$. Knowing that

$$
\int_{-4}^{4} \rho(s) s^{2k}\, ds = \binom{2k}{k}^2
$$

for $\rho(s) = (2\pi^2)^{-1} K(1 - s^2/16)$, where K denotes the elliptic integral, we would like to determine a function $\rho^{(\lambda)}(s)$ such that

$$
\int_{-2(1+\tilde{\lambda})}^{2(1+\tilde{\lambda})} \rho^{(\lambda)}(s) s^{2k}\, ds = \binom{2k}{k} \sum_{k_1=0}^{k} \binom{k}{k_1}^2 \tilde{\lambda}^{2k_1}
$$

as in (30). The special case $\tilde{\lambda} = 1$ clearly corresponds to the aforementioned formula.

We interpret the desired function $\rho^{(\lambda)}(s)$ as the density of a random variable with support $[-2(1+\tilde{\lambda}), 2(1+\tilde{\lambda})]$ that is symmetric (so that the odd-order moments are 0) and has $2k$th moment

$$M_{2k} = \binom{2k}{k} \sum_{k_1=0}^{k} \binom{k}{k_1}^2 \tilde{\lambda}^{2k_1}.$$

The moment generating function associated with this random variable is

$$\begin{aligned}
\sum_{k=0}^{\infty} \frac{M_{2k}}{(2k)!} x^{2k} &= \sum_{k=0}^{\infty} \binom{2k}{k} \sum_{k_1=0}^{k} \binom{k}{k_1}^2 \tilde{\lambda}^{2k_1} \frac{x^{2k}}{(2k)!} \\
&= \sum_{k_1=0}^{\infty} \sum_{k=k_1}^{\infty} \binom{2k}{k} \binom{k}{k_1}^2 \tilde{\lambda}^{2k_1} \frac{x^{2k}}{(2k)!} \\
&= \sum_{k_1=0}^{\infty} \frac{\tilde{\lambda}^{2k_1}}{k_1!^2} \sum_{k=k_1}^{\infty} \frac{1}{(k-k_1)!^2} x^{2k} \\
&= \sum_{k_1=0}^{\infty} \frac{\tilde{\lambda}^{2k_1}}{k_1!^2} \sum_{j=0}^{\infty} \frac{1}{j!^2} x^{2(k_1+j)} \\
&= \sum_{k_1=0}^{\infty} \frac{\tilde{\lambda}^{2k_1} x^{2k_1}}{k_1!^2} \sum_{j=0}^{\infty} \frac{x^{2j}}{j!^2} \\
&= I(2\tilde{\lambda}x) I(2x),
\end{aligned}$$

where I denotes the 0-th order modified Bessel function of the first kind. Thus the random variable whose density $\rho^{(\lambda)}(s)$ we would like to determine is the convolution of two random variables with moment generating functions $I(2\tilde{\lambda}x)$ and $I(2x)$, respectively.

Now note that $I(2x)$ is exactly the moment generating function of an arcsine distribution on the interval $[-2, 2]$,

$$\int_{-2}^{2} \frac{e^{sx}}{\pi\sqrt{4-s^2}}\, ds = I(2x),$$

and likewise $I(2\tilde{\lambda}x)$ is the moment generating function of an arcsine distribution on the interval $[-2\tilde{\lambda}, 2\tilde{\lambda}]$,

$$\int_{-2\tilde{\lambda}}^{2\tilde{\lambda}} \frac{e^{sx}}{\pi\sqrt{4\tilde{\lambda}^2-s^2}}\, ds = I(2\tilde{\lambda}x).$$

Therefore $\rho^{(\lambda)}(s)$ must be the convolution of the two densities $h_1(s) = (\pi\sqrt{4-s^2})^{-1}$ ($s \in [-2, 2]$, otherwise $h_1(s) = 0$) and $h_2(s) = (\pi\sqrt{4\tilde{\lambda}^2 - s^2})^{-1}$ [$s \in [-2\tilde{\lambda}, 2\tilde{\lambda}]$, otherwise $h_2(s) = 0$], which is

$$\rho^{(\lambda)}(s) = \int_{-\infty}^{\infty} h_1(s-t) h_2(t)\, dt.$$

This reduces to several different cases:

- Case 1: $\tilde{\lambda} > 1$
  (1) if $s < -2 - 2\tilde{\lambda}$ or $s > 2 + 2\tilde{\lambda}$, then $\rho^{(\lambda)}(s) = 0$,
  (2) if $-2 - 2\tilde{\lambda} \le s < 2 - 2\tilde{\lambda}$, then

$$\rho^{(\lambda)}(s) = \pi^{-2} \int_{-2\tilde{\lambda}}^{s+2} \frac{1}{\sqrt{(4-(s-t)^2)(4\tilde{\lambda}^2 - t^2)}}\, dt,$$

  (3) if $2 - 2\tilde{\lambda} \le s \le 2\tilde{\lambda} - 2$, then

$$\rho^{(\lambda)}(s) = \pi^{-2} \int_{s-2}^{s+2} \frac{1}{\sqrt{(4-(s-t)^2)(4\tilde{\lambda}^2 - t^2)}}\, dt,$$

(4) if $2\tilde{\lambda} - 2 < s \le 2\tilde{\lambda} + 2$, then

$$\rho^{(\lambda)}(s) = \pi^{-2} \int_{s-2}^{2\tilde{\lambda}} \frac{1}{\sqrt{(4-(s-t)^2)(4\tilde{\lambda}^2 - t^2)}}\, dt.$$

- Case 2: $0 < \tilde{\lambda} < 1$

(1) if $s < -2 - 2\tilde{\lambda}$ or $s > 2 + 2\tilde{\lambda}$, then $\rho^{(\lambda)}(s) = 0$,
(2) if $-2 - 2\tilde{\lambda} \le s < 2\tilde{\lambda} - 2$, then

$$\rho^{(\lambda)}(s) = \pi^{-2} \int_{-2\tilde{\lambda}}^{s+2} \frac{1}{\sqrt{(4-(s-t)^2)(4\tilde{\lambda}^2 - t^2)}}\, dt,$$

(3) if $2\tilde{\lambda} - 2 \le s \le 2 - 2\tilde{\lambda}$, then

$$\rho^{(\lambda)}(s) = \pi^{-2} \int_{-2\tilde{\lambda}}^{2\tilde{\lambda}} \frac{1}{\sqrt{(4-(s-t)^2)(4\tilde{\lambda}^2 - t^2)}}\, dt,$$

(4) if $2 - 2\tilde{\lambda} < s \le 2\tilde{\lambda} + 2$, then

$$\rho^{(\lambda)}(s) = \pi^{-2} \int_{s-2}^{2\tilde{\lambda}} \frac{1}{\sqrt{(4-(s-t)^2)(4\tilde{\lambda}^2 - t^2)}}\, dt.$$

All these integrals can be expressed in terms of the complete elliptic integral $K(x)$ that appeared previously in (12) and (34).

For instance, consider the case that $\tilde{\lambda} > 1$ and $2\tilde{\lambda} - 2 < s \le 2\tilde{\lambda} + 2$. Then we can represent the density by

$$\rho^{(\lambda)}(s) = \pi^{-2} \int_{s-2}^{2\tilde{\lambda}} \frac{1}{\sqrt{(4-(s-t)^2)(4\tilde{\lambda}^2 - t^2)}}\, dt. \tag{A7}$$

Now consider the integral representation

$$\frac{1}{2\pi^2\sqrt{\tilde{\lambda}}} K\Big(\frac{(2\tilde{\lambda}+2)^2 - s^2}{16\tilde{\lambda}}\Big) = \frac{1}{4\pi^2\sqrt{\tilde{\lambda}}} \int_{-1}^{1} \frac{dx}{\sqrt{(1-x^2)(1 - \frac{(2\tilde{\lambda}+2)^2 - s^2}{16\tilde{\lambda}} x^2)}}.$$

The rational substitution

$$x = \frac{8\tilde{\lambda} - 8\tilde{\lambda}^2 - 2\tilde{\lambda}s^2 + 4\tilde{\lambda}st + 2t^2 - 2\tilde{\lambda}t^2}{4\tilde{\lambda}^2 s + 4t - 4\tilde{\lambda}^2 t - s^2 t + st^2}$$

transforms this (as one readily checks) to the expression in (A7). Thus we have

$$\rho^{(\lambda)}(s) = \frac{1}{2\pi^2\sqrt{\tilde{\lambda}}} K\Big(\frac{(2\tilde{\lambda}+2)^2 - s^2}{16\tilde{\lambda}}\Big)$$

in this case. The other cases are treated in a similar fashion. We end up with the following general formula which holds for all positive values of $\tilde{\lambda}$:

$$\rho^{(\lambda)}(s) = \begin{cases} 0, & |s| \ge 2 + 2\tilde{\lambda}, \\ \frac{1}{2\pi^2\sqrt{\tilde{\lambda}}} K\Big(\frac{(2\tilde{\lambda}+2)^2 - s^2}{16\tilde{\lambda}}\Big), & |2\tilde{\lambda} - 2| \le |s| < 2\tilde{\lambda} + 2, \\ \frac{2}{\pi^2\sqrt{(2\tilde{\lambda}+2)^2 - s^2}} K\Big(\frac{16\tilde{\lambda}}{(2\tilde{\lambda}+2)^2 - s^2}\Big), & |s| < 2\tilde{\lambda} - 2. \end{cases}$$

We remark that the limiting case $\tilde{\lambda} = 0$ yields the density of an arcsine distribution on $[-2, 2]$.

APPENDIX C: EQUATION (32) CAN BE OBTAINED AS IN REF. 1

In order to reproduce from the lattice walks formulation in Ref. 1 the results obtained above for $\lambda \neq 2$, all that is needed is to consider lattice walks with asymmetric probability jumps on the horizontal axis versus the vertical axis in a ratio λ. One sets in the generating function $A(x_1, x_2, y_1, y_2, \mathrm{Q})$ [defined in Eq. (10) of Ref. 1] $x_1 \to zx$, $x_2 \to z/x$, $y_1 \to (\lambda/2)zy$, and $y_2 \to (\lambda/2)z/y$ and looks at the coefficients with vanishing exponents in x and y (i.e., $m_1 - m_2 = 0$ and $l_1 - l_2 = 0$) and exponent n in z (i.e., $m_1 + m_2 + l_1 + l_2 = n$),

$$\left[x^0 y^0\right] A(zx, z/x, (\lambda/2)zy, (\lambda/2)z/y) = \left[x^0 y^0\right] \frac{\begin{vmatrix} 1 & -z/x & 0 & \cdots & 0 & -zx \\ 1 & c_1^{(\lambda)} & -z/x & \cdots & 0 & 0 \\ 1 & -zx & c_2^{(\lambda)} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & c_{q-2}^{(\lambda)} & -z/x \\ 1 & 0 & 0 & \cdots & -zx & c_{q-1}^{(\lambda)} \end{vmatrix}}{\begin{vmatrix} c_0^{(\lambda)} & -z/x & 0 & \cdots & 0 & -zx \\ -zx & c_1^{(\lambda)} & -z/x & \cdots & 0 & 0 \\ 0 & -zx & c_2^{(\lambda)} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2}^{(\lambda)} & -z/x \\ -z/x & 0 & 0 & \cdots & -zx & c_{q-1}^{(\lambda)} \end{vmatrix}}, \tag{A8}$$

where $c_k^{(\lambda)} = 1 - (\lambda/2)z(\mathrm{Q}^k y + \mathrm{Q}^{-k} y^{-1})$ with $\mathrm{Q} = e^{2i\pi p/q}$.

As in Ref. 1, the denominator has the form

$$\Delta(zx, z/x, (\lambda/2)zy, (\lambda/2)z/y) = 1 - z^q (x^q + x^{-q} + (\lambda/2)^q (y^q + y^{-q})) + V(z^2, (\lambda/2)^2 z^2).$$

For $x = y = 1$, we get

$$\Delta(z, z, (\lambda/2)z, (\lambda/2)z) = 1 - z^q (2 + 2(\lambda/2)^q) + V(z^2, (\lambda/2)^2 z^2)$$

so that

$$\begin{aligned} &\Delta(zx, z/x, (\lambda/2)zy, (\lambda/2)z/y) \\ &\qquad = \Delta(z, z, (\lambda/2)z, (\lambda/2)z) + z^q (2 + 2(\lambda/2)^q) - z^q (x^q + x^{-q} + (\lambda/2)^q (y^q + y^{-q})). \end{aligned}$$

On the other hand, recall that both the polynomial $b_{p/q}^{(\lambda)}(z) = -\sum_{j=0}^{[\frac{q}{2}]} a_{p/q}^{(\lambda)}(2j) z^{2j}$ defined in (25) and the matrix $m_{p/q}^{(\lambda)}(e, 0, 0)$ defined in (23) are related by (26). Since also

$$\Delta(z, z, (\lambda/2)z, (\lambda/2)z) = (-z)^q \det\left(m_{p/q}^{(\lambda)}(1/z, 0, 0)\right),$$

it follows that

$$\Delta(z, z, (\lambda/2)z, (\lambda/2)z) = b_{p/q}^{(\lambda)}(z) - z^q (2 + 2(\lambda/2)^q)$$

and finally

$$\Delta(zx, z/x, (\lambda/2)zy, (\lambda/2)z/y) = b_{p/q}^{(\lambda)}(z) - z^q (x^q + x^{-q} + (\lambda/2)^q (y^q + y^{-q})).$$

Accordingly, and as shown in the Appendix of Ref. 1 [see the proof of (18)], the numerator at order x^0y^0 ends up being expressed only in terms of $b^{(\lambda)}_{p/q}(z)$,

$$\left[x^0y^0\right]\begin{vmatrix} 1 & -z/x & 0 & \cdots & 0 & -zx \\ 1 & c_1^{(\lambda)} & -z/x & \cdots & 0 & 0 \\ 1 & -zx & c_2^{(\lambda)} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & c_{q-2}^{(\lambda)} & -z/x \\ 1 & 0 & 0 & \cdots & -zx & c_{q-1}^{(\lambda)} \end{vmatrix} = b^{(\lambda)}_{p/q}(z) - \frac{z}{q} b^{(\lambda)}_{p/q}(z)'.$$

Finally (A8) rewrites as

$$\left[x^0y^0\right]A(zx, z/x, (\lambda/2)zy, (\lambda/2)z/y) = [x^0y^0]\frac{b^{(\lambda)}_{p/q}(z) - \frac{z}{q}b^{(\lambda)}_{p/q}(z)'}{b^{(\lambda)}_{p/q}(z) - z^q(x^q + x^{-q} + (\lambda/2)^q(y^q + y^{-q}))}$$
$$= \left(1 - \frac{zb^{(\lambda)}_{p/q}(z)'}{qb^{(\lambda)}_{p/q}(z)}\right)\sum_{k\geq 0}\left(\frac{z^q}{b^{(\lambda)}_{p/q}(z)}\right)^k [x^0y^0]\left(x^q + x^{-q} + (\lambda/2)^q(y^q + y^{-q})\right)^k$$

which yields the generating function (32) for the traces $\mathrm{Tr}\left(H^{(\lambda)}_{2\pi p/q}\right)^n$; we have

$$\left[x^0y^0\right](x^q + x^{-q} + (\lambda/2)^q(y^q + y^{-q}))^k = \left[x^0y^0\right]\sum_{k_1+k_2+k_3+k_4=k}\binom{k}{k_1, k_2, k_3, k_4}(\lambda/2)^{q(k_1+k_2)}x^{q(k_3-k_4)}y^{q(k_1-k_2)}$$
$$= \sum_{\substack{k_1+k_3=k/2 \\ k \text{ even}}}\binom{k}{k_1, k_1, k_3, k_3}(\lambda/2)^{2qk_1}$$
$$= \binom{k}{k/2}\sum_{k_1=0}^{k/2}\binom{k/2}{k_1}^2(\lambda/2)^{2qk_1}.$$

The coefficient at order x^0y^0 of $(x^q + x^{-q} + (\lambda/2)^q(y^q + y^{-q}))^k$ is $\binom{k}{k/2}\sum_{k_1=0}^{k/2}\binom{k/2}{k_1}^2(\lambda/2)^{2qk_1}$ if k is even and 0 otherwise so that finally

$$\sum_{n\geq 0, n \text{ even}}\mathrm{Tr}(H^{(\lambda)}_{2\pi p/q})^n z^n = \left(1 - \frac{zb^{(\lambda)}_{p/q}(z)'}{qb^{(\lambda)}_{p/q}(z)}\right)\sum_{k\geq 0}\left(\frac{z^q}{b^{(\lambda)}_{p/q}(z)}\right)^{2k}\binom{2k}{k}\sum_{k_1=0}^{k}\binom{k}{k_1}^2(\lambda/2)^{2qk_1}.$$

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Chapter

4 THOULESS BANDWIDTH FORMULA IN THE HOFSTADTER MODEL

In the previous chapter, we used the Hofstadter point trace formula eq. (3.15) as a tool to get an expression for the moments of the Hofstadter Hamiltonian eq. (2.23). On the other hand, Thouless [20–22] in the 80's and 90's focused on the total bandwidth of the Hofstadter model and its scaling in the limit $q \to \infty$. The bandwidth is the addition of the width of all the individual bands. It is defined in our notation as

$$(-1)^{q+1} \sum_{r=1}^{q} (-1)^r \left(E_r(-4) - E_r(4) \right) \tag{4.1}$$

where $E_r(\pm 4)$ are the solutions of eq. (3.10) with $s = \pm 4$, the edges of each band (see fig. 4.2, simple examples of $q = 3$ and $q = 4$). In the next section, we will justify eq. (4.1). So a natural question arises, using Thouless's method can we calculate the bandwidth n-th moment, defined as

$$(-1)^{q+1} \sum_{r=1}^{q} (-1)^r \left(E_r(-4) - E_r(4) \right)^n \tag{4.2}$$

It turns out computing this n-th moment in the scaling limit $q \to \infty$ is quite difficult. We will discuss this challenge and the associated difficulties in the following sections. We are going to argue that we can generalize Thouless's approach to

$$(-1)^{q+1} \sum_{r=1}^{q} (-1)^r \left(E_r(-4)^n - E_r(4)^n \right), \tag{4.3}$$

which is a truncation of eq. (4.2). The results are published in [23] which is the Article 3 inserted at the end of this chapter. We will come back to the bandwidth n-th moment at the end of this chapter.

4.1 Introduction

As explained in the previous chapter, for a given rational flux $\gamma = 2\pi p/q$, the characteristic polynomial $E^q b_{p/q}(1/E)$ defined in eq. (3.8) has q individual bands (see the simple cases $q = 3$ and $q = 4$ in fig. 4.2). Thus, the bandwidth is defined in terms of the $2q$ edges of the bands, that we denote as $E_r(4)$ and $E_r(-4)$ with $r = 1, 2, \ldots, q$. They are the solutions of

$$E^q b_{p/q}(1/E) = 4 \quad \text{and} \quad E^q b_{p/q}(1/E) = -4,$$

respectively. Moreover, we order the edges such that

$$E_1(4) \leq E_2(4) \leq \ldots \leq E_q(4) \quad \text{and} \quad E_1(-4) \leq E_2(-4) \leq \ldots \leq E_q(-4).$$

The bandwidth is then defined as in eq. (4.1)

$$(-1)^{q+1}\sum_{r=1}^{q}(-1)^r\left(E_r(-4)-E_r(4)\right).$$

The $(-1)^r$ and the $(-1)^{q+1}$ factors in this equation are here to keep every term in the summation positive. Because of the $(-1)^r$ factor, a difficulty arises: the plus and minus signs of $E_r(4)$ and $E_r(-4)$ alternate with each other, so one had to specify the ordering of $E_r(4)$ and $E_r(-4)$ (see the examples in fig. 4.2). It is difficult to compute such a non-symmetric sum. However, Thouless managed to overcome this difficulty and was able to compute the asymptotic behavior of the bandwidth when q goes to infinity :

$$\lim_{q\to\infty} q(-1)^{q+1}\sum_{r=1}^{q}(-1)^r\left(E_r(-4)-E_r(4)\right)=\frac{32}{\pi}G \tag{4.4}$$

This formula tells us that the Hofstadter spectral measure scaled as $\frac{32}{\pi}G/q$ where $G=\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)^2}$ is the Catalan's constant. We will detail Thouless's method in the next section.

4.2 Bandwidth calculation: Thouless's method

First of all, in the following, let us focus on the case q odd. The advantage of q being odd is that there exists a symmetry property of the band edges

$$E_r(-4)=-E_{q+1-r}(4).$$

Therefore, using this symmetry, eq. (4.1) is reduced to the $E_r(4)$'s:

$$\sum_{r=1}^{q}(-1)^r\left(E_r(-4)-E_r(4)\right)=-2\sum_{r=1}^{q}(-1)^r E_r(4).$$

Also, from eq. (3.7), we know that $E_r(4)$ are the roots of $\det\left(m_{p/q}(E,0,0)\right)=0$.

Key points

Thouless made two crucial observations to be able to obtain eq. (4.4):

- The first one is the factorization of $\det\left(m_{p/q}(E,0,0)\right)$. This determinant can be factorized into the product of the determinants of two submatrices $m^{++}_{p/q}(E)$ and $m^{--}_{p/q}(E)$:

$$\det\left(m_{p/q}(E,0,0)\right)=\det\left(m^{++}_{p/q}(E)\right)\det\left(m^{--}_{p/q}(E)\right) \tag{4.5}$$

  where

$$m^{++}_{p/q}(E)=\begin{pmatrix} E-2 & 2 & 0 & \cdots & 0 & 0\\ 1 & E-2\cos\left(2\pi\frac{p}{q}\right) & 1 & \cdots & 0 & 0\\ 0 & 1 & () & \cdots & 0 & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & 0 & \cdots & () & 1\\ 0 & 0 & 0 & \cdots & 1 & E-2\cos\left(\frac{q-1}{2}\frac{2\pi p}{q}\right)-1 \end{pmatrix},$$

$$m^{--}_{p/q}(E) = \begin{pmatrix} E-2\cos\left(2\pi\frac{p}{q}\right) & 1 & 0 & \cdots & 0 & 0 \\ 1 & E-2\cos\left(4\pi\frac{p}{q}\right) & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ 0 & 0 & 0 & \cdots & 1 & E-2\cos\left(\frac{q-1}{2}\frac{2\pi p}{q}\right)+1 \end{pmatrix}.$$

$m^{++}_{p/q}(E)$ and $m^{--}_{p/q}(E)$ are tridiagonal matrices with size $(q+1)/2$ and $(q-1)/2$ respectively. So the eigenvalues $E_r(4)$ split into two parts: E_r^{++} and E_r^{--} which are the eigenvalues of $m^{++}_{p/q}(E)$ and $m^{--}_{p/q}(E)$ respectively.

- Another critical observation is that the positive eigenvalues E_r^{++} alternate with E_r^{--}, and so do the negative eigenvalues, although the order is reversed (see the fig. 4.1). Thus, the bandwidth can be written in terms of E_r^{++} and E_r^{--} as

$$-2\sum_{r=1}^{q}(-1)^r E_r(4) = 2\left(\sum_{r=1}^{\frac{q+1}{2}}|E_r^{++}| - \sum_{r=1}^{\frac{q-1}{2}}|E_r^{--}|\right).$$

Then the bandwidth calculation becomes possible because the equation above is the difference between two symmetric sums. The price to be paid is the absolute value in front of E_r^{++} and E_r^{--}. In the following, we will give some technical details how to calculate the bandwidth in this way.

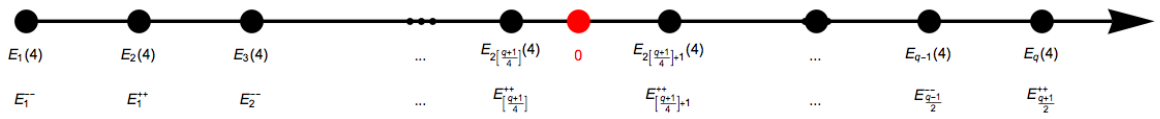

Figure 4.1: *the $E_r(4)$ split into E_r^{++} and E_r^{--}*

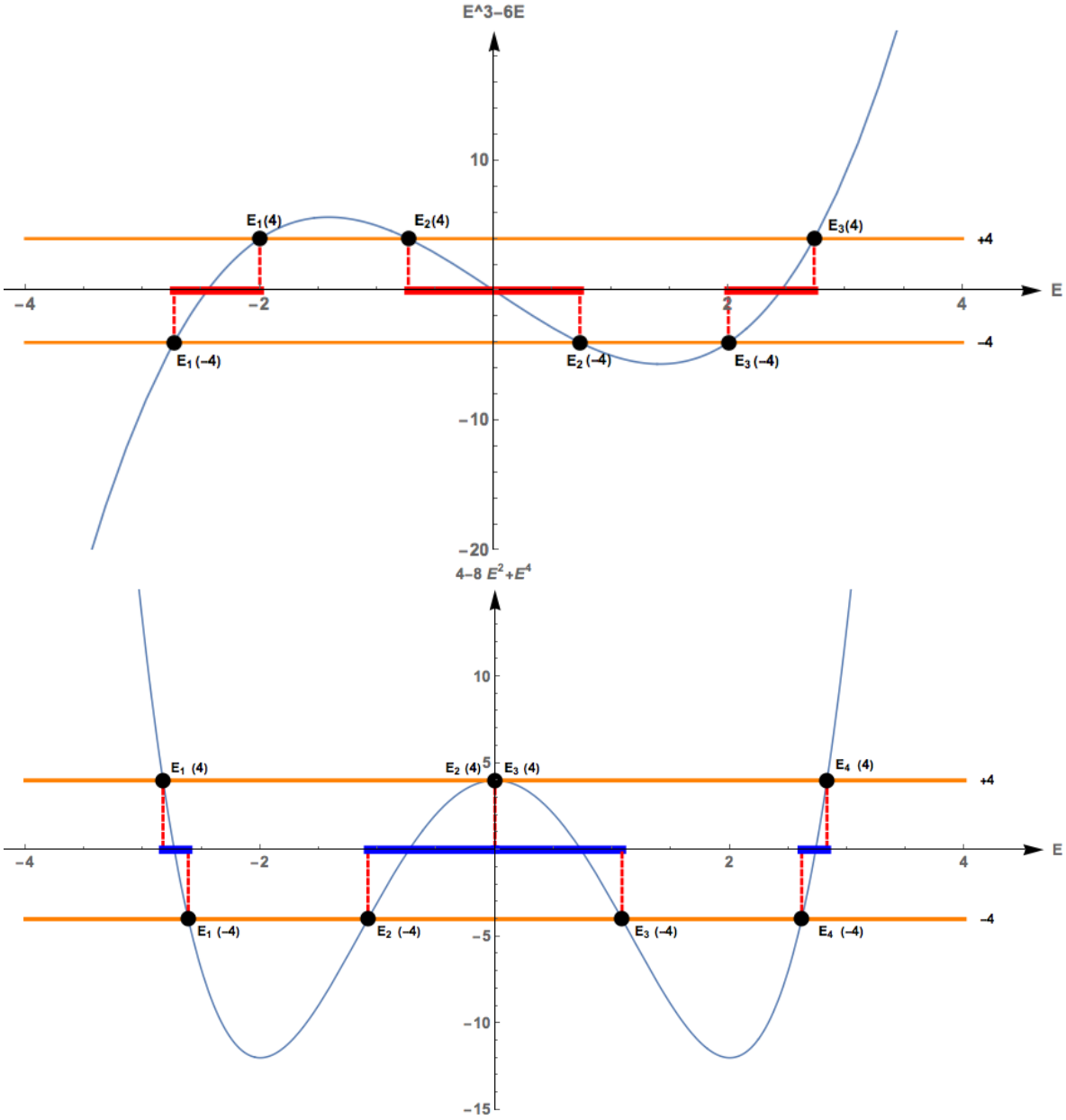

Figure 4.2: *two simple examples: the top figure represents the case $p = 1$ and $q = 3$, its characteristic polynomial is $6E - E^3$, the three red segments are the three energy bands, each band do not overlap. The six black dots correspond to the edges of bands. Its bandwidth is $-E_1(-4) + E_1(4) - E_2(4) + E_2(-4) - E_3(-4) + E_3(4)$. The bottom figure corresponds to the case $p = 1$ and $q = 4$, its characteristic polynomial is $E^4 - 8E^2 + 4$, the four blue segments are the four energy bands, two central bands touch each other in zero energy. Its bandwidth is $-E_1(4) + E_1(-4) - E_2(-4) + E_2(4) - E_3(4) + E_3(-4) - E_4(-4) + E_4(4)$.*

Technics

In order to calculate the absolute value of a, we introduce the integral

$$\frac{2i}{\pi}\int_{-ix}^{ix}\left(\frac{z}{z-a}-1\right)dz=\frac{4a}{\pi}\arctan\left(\frac{x}{a}\right),$$

which contains an arctangent function in the RHS, and in the limit of x goes to infinity, gives the absolute value of a:

$$\lim_{x\to\infty}\frac{4a}{\pi}\arctan\left(\frac{x}{a}\right)=2|a|.$$

In the same limit, by partial integration:

$$\lim_{x\to\infty}\int_{-ix}^{ix}\left(\frac{z}{z-a}-1\right)dz=\lim_{x\to\infty}\int_{-ix}^{ix}\left(-\log\frac{z-a}{z}\right)dz.$$

By using the identities above, we get

$$2\left(\sum_{r=1}^{\frac{q+1}{2}}|E_r^{++}|-\sum_{r=1}^{\frac{q-1}{2}}|E_r^{--}|\right)=\frac{2i}{\pi}\lim_{x\to\infty}\int_{-ix}^{ix}\left(\frac{\det\left(m_{p/q}^{--}(z)\right)}{\det\left(m_{p/q}^{++}(z)\right)}\right)dz. \tag{4.6}$$

So far, all the equations above are exacts. To make further progress for large q, what Thouless did is to make further algebraic manipulations: E_r^{++} are the eigenvalues of

$$a_{n-1}+\left(2\cos\left(\frac{2\pi p}{q}n\right)+\delta(n-(q-1)/2)\right)a_n+a_{n+1}=E^{++}a_n \tag{4.7}$$

with $0\leq n\leq(q-1)/2$ and the boundary conditions $a_{(q+1)/2}=a_{(q-1)/2}$ and $a_1=a_{-1}$. E_r^{--} are the eigenvalues of

$$b_{n-1}+\left(2\cos\left(\frac{2\pi p}{q}n\right)-\delta(n-(q-1)/2)\right)b_n+b_{n+1}=E^{--}b_n \tag{4.8}$$

with $1\leq n\leq(q-1)/2$ and the boundary condition $b_0=0$. From the two recurrence relations above, one notices that the ratio of determinants in eq. (4.6) can be written in terms of particular solutions a_n and b_n of eq. (4.7) and eq. (4.8):

$$\frac{\det\left(m_{p/q}^{--}(z)\right)}{\det\left(m_{p/q}^{++}(z)\right)}=\frac{a_0}{a_{-1}-a_1}\frac{b_{(q+1)/2}+b_{(q-1)/2}}{b_{(q+1)/2}-b_{(q-1)/2}}.$$

At the limit of $q\to\infty$, one can make a continuum approximation for eq. (4.7) and eq. (4.8), the gain is the transition from difference to differential equations. Thus, a_n and b_n are solutions of parabolic cylinder functions, from [24, pp. 678-693], the approximations of the solutions are

$$a_n\approx(-1)^nE\left(-zq/(4\pi),\sqrt{4\pi/q}n\right)$$

$$b_n\approx E^*\left(zq/(4\pi),\sqrt{4\pi/q}(q/2-n)\right)$$

with $E(a,x)=k^{-1/2}W(a,x)+ik^{1/2}W(a,-x)$, $E^*(a,x)=k^{-1/2}W(a,x)-ik^{1/2}W(a,-x)$ and $W(a,x)$ are functions involving gamma functions (see the section 19.17. Standard Solutions in [24]). Therefore, with the change of the variable $y=qz/(8\pi i)$, the ratio between the determinants in the limit of $q\to\infty$ is rewritten in terms of the logarithm of the ratio of gamma functions:

$$\lim_{q\to\infty}2q\left(\sum_{r=1}^{\frac{q+1}{2}}|E_r^{++}|-\sum_{r=1}^{\frac{q-1}{2}}|E_r^{--}|\right)=32\int_0^\infty\log\left(\frac{\Gamma(3/4+y)^2}{y\Gamma(1/4+y)^2}\right)dy$$

This last integral gives

$$\lim_{q\to\infty} q\left(\sum_{r=1}^{q}(-1)^r\left(E_r(-4)-E_r(4)\right)\right)=\frac{4}{\pi}\left(\psi^{(1)}\left(\frac{1}{4}\right)-\pi^2\right) \tag{4.9}$$

which is a rewriting of eq. (4.4) ($\psi^{(1)}\left(\frac{1}{4}\right)$ is the polygamma function of order 1).

4.3 Generalization of Thouless's formula

The previous section reviewed the method used by Thouless for calculating the bandwidth of the Hofstadter model. In this section, we now detail what we did by generalizing Thouless's method to compute the truncated n-th moment eq. (4.3). First, as mentioned above, our goal was to calculate the bandwidth n-th moment eq. (4.2), which in the case q odd and n odd is

$$\sum_{r=1}^{q}(-1)^r\left(E_r(-4)-E_r(4)\right)^n. \tag{4.10}$$

Comparing to Thouless's case when $n=1$, there is not only the $(-1)^r$ in the front, but moreover, the difference between $E_r(-4)$ and $E_r(4)$ at the power n, which cannot be decomposed into two symmetric sums as before. So we leave aside for the time being the task of calculating this bandwidth n-th moment, and focus on the truncation of eq. (4.10) (we will come back in the conclusion to the n-th moment bandwidth). We have defined this truncated n-th moment in eq. (4.3), as:

$$\sum_{r=1}^{q}(-1)^r\left(E_r(-4)^n-E_r(4)^n\right).$$

It vanishes when n is even because of the symmetry $E_r(4)=-E_{q+1-r}(-4)$. Thus, in the following we concentrate on the case q odd and n odd. Also, thanks again to the symmetry and the factorization used previously, it can be written as

$$\begin{aligned}\sum_{r=1}^{q}(-1)^r\left(E_r(-4)^n-E_r(4)^n\right) &\overset{E_r(4)=-E_{q+1-r}(-4)}{=} -2\sum_{r=1}^{q}(-1)^r E_r(4)^n\\ &\overset{\text{factorization}}{=} 2\left(\sum_{r=1}^{\frac{q+1}{2}}|E_r^{++}|^n-\sum_{r=1}^{\frac{q-1}{2}}|E_r^{--}|^n\right)\end{aligned}$$

The second equation in the RHS is again the difference between two symmetric sums of absolute values with a higher order exponent n. Now by following the same logic as in the case $n=1$, some identities can be used to calculate the $|E_r^{\pm\pm}|^n$, which are analogous to the identities mentioned previously but with an exponent n:

$$\frac{2i}{\pi}\int_{-ix}^{ix}\left(\frac{z^n}{z-a}-\sum_{k=0}^{n-1}a^k z^{n-1-k}\right)dz=\frac{4a^n}{\pi}\arctan\left(\frac{x}{a}\right),$$

$$\lim_{x\to\infty}\frac{4a^n}{\pi}\arctan\left(\frac{x}{a}\right)=2|a^n|$$

and

$$\lim_{x\to\infty}\int_{-ix}^{ix}\left(\frac{z^n}{z-a}-\sum_{k=0}^{n-1}a^k z^{n-1-k}\right)dz=\lim_{x\to\infty}\int_{-ix}^{ix}-nz^{n-1}\left(\log\frac{z-a}{z}+\sum_{k=1}^{n-1}\frac{a^k}{kz^k}\right)dz. \tag{4.11}$$

Comparing with the case $n = 1$, instead of z we have z^n in the integral, and the corresponding sums (with index k) make sure that the integrals are finite. Replacing a by E_r^{++} and E_r^{--}, one gets

$$2\left(\sum_{r=1}^{\frac{q+1}{2}}|E_r^{++}|^n-\sum_{r=1}^{\frac{q-1}{2}}|E_r^{--}|^n\right)=\frac{2i}{\pi}\lim_{x\to\infty}\int_{-ix}^{ix}nz^{n-1}\left(\log\left(\frac{z\det\left(m_{p/q}^{--}(z)\right)}{\det\left(m_{p/q}^{++}(z)\right)}\right)-\sum_{k=1}^{n-1}\frac{\sum_{r=1}^{\frac{q+1}{2}}(E_r^{++})^k-\sum_{r=1}^{\frac{q-1}{2}}(E_r^{--})^k}{kz^k}\right)dz. \tag{4.12}$$

In the RHS of eq. (4.12), $-z^{n-1}\sum_{k=1}^{n-1}\left(\frac{\sum_{r=1}^{\frac{q+1}{2}}(E_r^{++})^k-\sum_{r=1}^{\frac{q-1}{2}}(E_r^{--})^k}{kz^k}\right)$ does cancel the positive or null exponents in the expansion around $z=\infty$ in the logarithm term $z^{n-1}\log\left(\frac{z\det\left(m_{p/q}^{--}(z)\right)}{\det\left(m_{p/q}^{++}(z)\right)}\right)$ to keep the integral finite. When q goes to infinity, as in the case $n = 1$, making further algebraic manipulation and taking the same continuum approximation, with the change of variable $y = qz/(8i\pi)$, we get

$$\lim_{q\to\infty}2q^n\left(\sum_{r=1}^{\frac{q+1}{2}}|E_r^{++}|^n-\sum_{r=1}^{\frac{q-1}{2}}|E_r^{--}|^n\right)=(8\pi i)^{n-1}32\int_0^{\infty}ny^{n-1}\left(\log\left(\frac{1}{y}\frac{\Gamma(3/4+y)^2}{\Gamma(1/4+y)^2}\right)+\sum_{k=2,k\text{ even}}^{n-1}\frac{E_k}{k4^ky^k}\right)dy \tag{4.13}$$

where the E_k's are the Euler numbers. To get eq. (4.13) from eq. (4.12), necessarily, we should have for k even

$$\lim_{q\to\infty}q^k\left(\sum_{r=1}^{\frac{q+1}{2}}|E_r^{++}|^k-\sum_{r=1}^{\frac{q-1}{2}}|E_r^{--}|^k\right)=(2\pi)^k|E_k| \tag{4.14}$$

This is due to the fact that in eq. (4.13), the polynomial $\sum_{k=2,k\text{ even}}^{n-1}E_k/(k4^k)y^{n-1-k}$ plays the same role as $\sum_{k=1}^{n-1}\left(\frac{\sum_{r=1}^{\frac{q+1}{2}}(E_r^{++})^k-\sum_{r=1}^{\frac{q-1}{2}}(E_r^{--})^k}{kz^{k-n+1}}\right)$ in eq. (4.12) to insure that the integral is finite. Indeed, the series expansion when y goes to infinity of $\log\left(\frac{1}{y}\frac{\Gamma(3/4+y)^2}{\Gamma(1/4+y)^2}\right)$ starts with the polynomial $-\sum_{k=2,k\text{ even}}^{n-1}\frac{E_k}{k4^ky^k}$ expressed in terms of the Euler numbers. See the proof in the appendix of Article 3. It is interesting to note that in order to compute the odd n truncated moment in eq. (4.3), one sees appearing in the RHS of eq. (4.12) the same truncated moment but now for k even, which in turn is given by eq. (4.14).

After computing the last integral of eq. (4.13), we get

$$\lim_{q\to\infty}q^n\left(\sum_{r=1}^{q}(-1)^r\left(E_r(-4)^n-E_r(4)^n\right)\right)=\frac{4}{\pi}\left((-1)^{n-1}\psi^{(n)}\left(\frac{1}{4}\right)-2^n(2^{n+1}-1)\zeta(n+1)n!\right) \tag{4.15}$$

which generalizes the Thouless's formula eq. (4.9) to n odd ($\psi^{(n)}$ is the polygamma function of order n).

4.4 Conclusion and opened issues

In this chapter, we generalized Thouless bandwidth formula eq. (4.4) to the truncated n-th moment eq. (4.15) for n odd. In the Article 3, we derived that for all n odd and n even,

$$\begin{aligned}
&\frac{4}{\pi}\left((-1)^{n-1}\psi^{(n)}\left(\frac{1}{4}\right) - 2^n(2^{n+1}-1)\zeta(n+1)n!\right) \\
&= \frac{2}{\pi}4^{n+1}n!\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)^{n+1}} \\
&= \frac{2}{\pi}n!\left(\zeta(n+1,\frac{1}{4}) - \zeta(n+1,\frac{3}{4})\right) \\
&= \frac{2}{\pi}(-1)^{n+1}\left(\psi^n\left(\frac{1}{4}\right) - \psi^n\left(\frac{3}{4}\right)\right)
\end{aligned} \tag{4.16}$$

coincides with eq. (4.15) when n is odd. And when n is even, it is q^n times twice the half spectrum n-th moment given by eq. (4.14) in terms of the Euler numbers.

Finally, returning to the bandwidth n-th moment defined in eq. (4.10) for n odd and q odd, we can rewrite it as

$$\begin{aligned}
\sum_{r=1}^{q}(-1)^r\left(E_r(-4)-E_r(4)\right)^n &= -2\sum_{k=0}^{(n-1)/2}\binom{n}{k}(-1)^k\sum_{r=1}^{q}(-1)^r E_r(-4)^k E_r(4)^{n-k} \\
&= -2\sum_{i=1}^{q}(-1)^r\left(E_r(-4)^n - E_r(4)^n\right) - 2\sum_{k=1}^{(n-1)/2}\binom{n}{k}(-1)^k\sum_{r=1}^{q}(-1)^r E_r(-4)^k E_r(4)^{n-k}
\end{aligned} \tag{4.17}$$

where the symmetry $E_r(4) = -E_{q+1-r}(-4)$ has again been used. The $k=0$ term in the RHS of eq. (4.17) is the truncated n-th moment obtained above eq. (4.15) with a q^n scaling. So the natural guess is that the bandwidth n-th moment should have the same scaling. Numerical simulations indicate that there exists a simple relation between the $k=0$ term and the $k\neq 0$ terms:

$$\begin{aligned}
\lim_{q\to\infty} -2q^n\sum_{r=1}^{q}(-1)^r E_r(-4)^k E_r(4)^{n-k} &= \frac{n-2k}{n}\lim_{q\to\infty} -2q^n\sum_{r=1}^{q}(-1)^r E_r(4)^n \\
&= \frac{n-2k}{n}\frac{4}{\pi}\left((-1)^{n-1}\psi^{(n)}\left(\frac{1}{4}\right) - 2^n(2^{n+1}-1)\zeta(n+1)n!\right)
\end{aligned} \tag{4.18}$$

with $k=1,\ldots,(n-1)/2$. Replacing the $k\neq 0$ terms in eq. (4.17) by eq. (4.18) and noticing that

$$\sum_{k=0}^{(n-1)/2}\binom{n}{k}(-1)^k\frac{n-2k}{n} = 0,$$

one concludes that in the $q\to\infty$ limit, the bandwidth n-th moment is such that

$$\lim_{q\to\infty} q^n\sum_{r=1}^{q}(-1)^r\left(E_r(-4)-E_r(4)\right)^n = 0$$

with n is odd and larger than 1, a fact which is also supported by numerical simulations. Similarly, when n is even, the bandwidth n-th moment now defined as

$$\sum_{r=1}^{q}\left(E_r(-4)-E_r(4)\right)^n$$

is such that $\lim_{q\to\infty} q^n \sum_{r=1}^{q} (E_r(-4) - E_r(4))^n = 0$.

Clearly, multiplying the sum in eq. (4.17) by q^n is insufficient, q^n is not the right scaling for the bandwidth n-th moment. In order to find the right scaling, we can turn to a multifractal analysis. The multifractal analysis was first innovated by Mandelbrot [25] and further developed by others [26], [27] and [28]. It is a useful tool to tell whether the scaling behavior is a power law for the statistical moments at different scales. If the statistical moments scale only depends on a single exponent, or equivalently on a linear function of the moments, the process is monofractal. If the scaling behavior by scale is a nonlinear function of the moments, the process is multifractal. In the following, we consider the multifractal dimension of the bandwidth n-th moment.

Consider a normalized quantity

$$\tilde{\mu}_r = \frac{\mu_r}{\sum_{i=1}^{q} \mu_i} \tag{4.19}$$

with

$$\mu_r = |E_r(-4) - E_r(4)|. \tag{4.20}$$

We want to test the asymptotic behavior of moments

$$\sum_{r=1}^{q} \tilde{\mu}_r^n \tag{4.21}$$

for large q, whether it is governed by a set of multifractal exponents τ_n defined by

$$\sum_{r=1}^{q} \tilde{\mu}_r^n \propto q^{-\tau_n} \tag{4.22}$$

which is related to the multifractal dimension $d_n(n-1) = \tau_n$. If the scaling behavior in eq. (4.22) is correct, then $\log\left(\sum_{r=1}^{q} \tilde{\mu}_r^n\right)$ is linear in $\log q$, the multifractal dimension d_n can be obtained in this way

$$d_n = \lim_{q\to\infty} \frac{-1}{n-1} \frac{\log\left(\sum_{r=1}^{q} \tilde{\mu}_r^n\right)}{\log q}. \tag{4.23}$$

Figure fig. 4.3 represents numerical simulations for eq. (4.23). The values of d_n are displayed as a function of n in fig. 4.3, and it seems multifractal because d_n is a non-trivial function of n. These results also confirm the conclusion we made before: q^n is not the right scaling for the bandwidth n-th moment. Because if q^n was the right scaling, then eq. (4.21) would be proportional to a constant, which leads to $d_n = 0$. This is apparently incompatible with the numerical results of eq. (4.23). However, as shown in fig. 4.3, for a given n, the values of d_n decrease with the values of q, when q increases, d_n becomes smaller, and converges very slowly. Thus, without comparing theoretical prediction, these numeric simulations can lead us to nowhere! We leave to further studies the question of finding a right scaling for the bandwidth n-th moment.

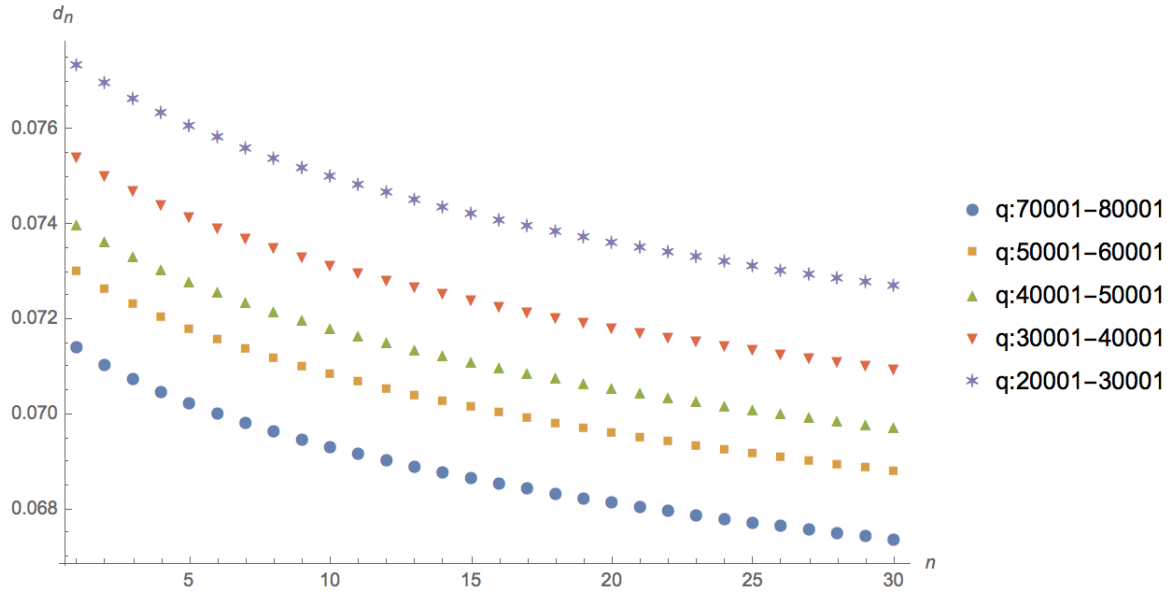

Figure 4.3: *the multifractal dimension of bandwidth n-th moment. Different colors represent different size q*

Article 3 :Thouless bandwidth formula in the Hofstadter model
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Thouless bandwidth formula in the Hofstadter model

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Abstract

We generalize the Thouless bandwidth formula to its nth moment. We obtain a closed expression in terms of polygamma, zeta and Euler numbers.

Keywords: Thouless bandwidth, nth moment, Hofstadter spectrum

(Some figures may appear in colour only in the online journal)

1. Introduction

In a series of stunning papers stretching over almost a decade [1], Thouless obtained a closed expression for the bandwidth of the Hofstadter spectrum [2] in the $q \to \infty$ limit. Here the integer q stands for the denominator of the rational flux $\gamma = 2\pi p/q$ of the magnetic field piercing a unit cell of the square lattice; the numerator p is taken to be 1 (or equivalently $q-1$). In the following, p will always be understood as equal to 1.

Let us recall that in the commensurate case where the lattice eigenstates $\Psi_{m,n} = \mathrm{e}^{\mathrm{i}nk_y}\Phi_m$ are q-periodic $\Phi_{m+q} = \mathrm{e}^{\mathrm{i}qk_x}\Phi_m$, with $k_x, k_y \in [-\pi, \pi]$, the Schrödinger equation

$$\Phi_{m+1} + \Phi_{m-1} + 2\cos(k_y + \gamma m)\Phi_m = e\Phi_m \tag{1}$$

reduces to the $q \times q$ secular matrix

$$m_{p/q}(e, k_x, k_y) = \begin{pmatrix} 2\cos(k_y) - e & 1 & 0 & \cdots & 0 & \mathrm{e}^{-\mathrm{i}qk_x} \\ 1 & 2\cos(k_y + \frac{2\pi p}{q}) - e & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ \mathrm{e}^{\mathrm{i}qk_x} & 0 & 0 & \cdots & 1 & 2\cos(k_y + (q-1)\frac{2\pi p}{q}) - e \end{pmatrix}$$

acting as

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$$m_{p/q}(e,k_x,k_y).\Phi = 0 \tag{2}$$

on the q-dimensional eigenvector $\Phi = \{\Phi_0, \Phi_1, \ldots, \Phi_{q-1}\}$. Thanks to the identity

$$\det(m_{p/q}(e,k_x,k_y)) = \det(m_{p/q}(e,0,0)) - 2(-1)^q(\cos(qk_x) - 1 + \cos(qk_y) - 1),$$

the eigenenergy equation $\det(m_{p/q}(e,k_x,k_y)) = 0$ rewrites [3] as

$$\det(m_{p/q}(e,0,0)) = 2(-1)^q(\cos(qk_x) - 1 + \cos(qk_y) - 1). \tag{3}$$

The polynomial

$$b_{p/q}(e) = -\sum_{j=0}^{[\frac{q}{2}]} a_{p/q}(2j)\mathrm{e}^{2j}$$

materializes in $\det(m_{p/q}(e,0,0))$

$$\det(m_{p/q}(e,0,0)) + 4(-1)^q = (-1)^q\mathrm{e}^q b_{p/q}(1/e) \tag{4}$$

so that (3) becomes

$$\mathrm{e}^q b_{p/q}(1/e) = 2(\cos(qk_x) + \cos(qk_y)).$$

The coefficients $a_{p/q}(2j)$'s (with $a_{p/q}(0) = -1$) in the polynomial $b_{p/q}(e)$ above are related to the Kreft coefficients [4] so that

$$a_{p/q}(2j) = (-1)^{j+1}\sum_{k_1=0}^{q-2j}\sum_{k_2=0}^{k_1}\cdots\sum_{k_j=0}^{k_{j-1}} 4\sin^2\left(\frac{\pi(k_1+2j-1)\,p}{q}\right)$$
$$\times 4\sin^2\left(\frac{\pi(k_2+2j-3)\,p}{q}\right)\ldots 4\sin^2\left(\frac{\pi(k_j+1)\,p}{q}\right).$$

How to get this explicit expression is explained in Kreft's paper.

We focus on the Hofstadter spectrum bandwidth defined in terms of the $2q$ edge-band energies $e_r(4)$ and $e_r(-4)$, $r = 1,2,\ldots,q$, solutions of

$$\mathrm{e}^q b_{p/q}(1/e) = 4 \text{ and } \mathrm{e}^q b_{p/q}(1/e) = -4,$$

respectively (see figures 1 and 2). If one specifies an ordering for the $e_r(4)$'s and the $e_r(-4)$'s

$$e_1(4) \leqslant e_2(4) \leqslant \ldots \leqslant e_q(4) \quad \text{and} \quad e_1(-4) \leqslant e_2(-4) \leqslant \ldots \leqslant e_q(-4)$$

the bandwidth is

$$(-1)^{q+1}\sum_{r=1}^{q}(-1)^r\big(e_r(-4) - e_r(4)\big). \tag{5}$$

The Thouless formula is obtained in the $q \to \infty$ limit as

$$\lim_{q\to\infty}(-1)^{q+1}q\sum_{r=1}^{q}(-1)^r\big(e_r(-4) - e_r(4)\big) = \frac{32}{\pi}\sum_{k=0}^{\infty}(-1)^k\frac{1}{(2k+1)^2} \tag{6}$$

(see also [5]). We aim to extend this result to the nth moment defined as

$$(-1)^{q+1}\sum_{r=1}^{q}(-1)^r\big(e_r^n(-4) - e_r^n(4)\big). \tag{7}$$

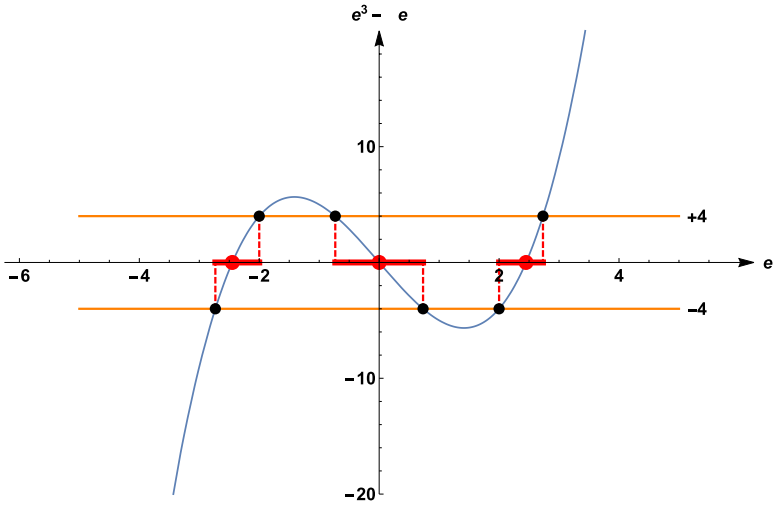

Figure 1. $p=1, q=3, \mathrm{e}^q b_{p/q}(1/e) = e^3 - 6e$: the three horizontal red segments are the energy bands; the three red dots are the mid-band energies; the six black dots are the ± 4 edge-band energies.

which is a natural generalization of (5): one can think of it as

$$n \int_{-4}^{4} \tilde{\rho}_{p/q}(e) \mathrm{e}^{n-1} \mathrm{d}e$$

where $\tilde{\rho}_{p/q}(e)$ is the indicator function with value 1 when $|\mathrm{e}^q b_{p/q}(1/e)| \leqslant 4$ and 0 otherwise. Let us stress that the bandwidth nth moment defined for n odd as

$$(-1)^{q+1} \sum_{r=1}^{q} (-1)^r \big(e_r(-4) - e_r(4)\big)^n, \tag{8}$$

is of particular interest. We will come back to this moment in the conclusion.

Trivially (7) vanishes when n is even—we will see later how to give a non-trivial meaning to the nth moment in this case. Therefore, we focus on (7) when n is odd and, additionally, when q is odd, in which case it simplifies further to

$$-2 \sum_{r=1}^{q} (-1)^r e_r^n(4) = 2 \sum_{r=1}^{q} (-1)^r e_r^n(-4) \tag{9}$$

thanks to the symmetry $e_r(-4) = -e_{q+1-r}(4)$. As said above, the $e_r(4)$'s are the roots of $\mathrm{e}^q b_{p/q}(1/e) = 4$ that is, by the virtue of (4), those of

$$\det(m_{p/q}(e,0,0)) = 0.$$

2. The first moment: Thouless formula

The key point in the observation of Thouless [1] is that if evaluating the first moment rewritten in (9) as $-2\sum_{r=1}^{q}(-1)^r e_r(4)$ when q is odd seems at first sight intractable, still, thanks to:

- $\det(m_{p/q}(e,0,0))$ factorizing as

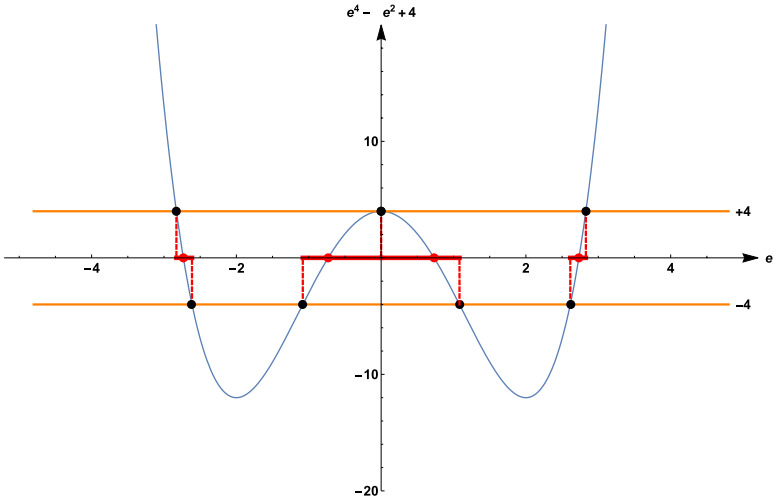

Figure 2. $p=1, q=4, \mathrm{e}^{q} b_{p/q}(1/e) = e^4 - 8e^2 + 4$: the four horizontal red segments are the energy bands; the four red dots are the mid-band energies; the eight black dots are the ± 4 edge-band energies—there are two degenerate dots located at the center.

$$\det(m_{p/q}(e,0,0)) = -\det(m^{++}_{p/q}(e))\det(m^{--}_{p/q}(e))$$

where

$$m^{++}_{p/q}(e) = \begin{pmatrix} e-2 & 2 & 0 & \cdots & 0 & 0 \\ 1 & e-2\cos(\frac{2\pi p}{q}) & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ 0 & 0 & 0 & \cdots & 1 & e-2\cos(\frac{q-1}{2}\frac{2\pi p}{q})-1 \end{pmatrix}$$

$$m^{--}_{p/q}(e) = \begin{pmatrix} e-2\cos(\frac{2\pi p}{q}) & 1 & 0 & \cdots & 0 & 0 \\ 1 & e-2\cos(\frac{4\pi p}{q}) & 1 & \cdots & 0 & 0 \\ 0 & 1 & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & 1 \\ 0 & 0 & 0 & \cdots & 1 & e-2\cos(\frac{q-1}{2}\frac{2\pi p}{q})+1 \end{pmatrix}$$

are matrices of size $(q+1)/2$ and $(q-1)/2$, respectively, so that the $e_r(4)$'s split in two packets e_r^{++}, $r=1,2,\ldots,(q+1)/2$, the roots of $\det(m^{++}_{p/q}(e))=0$ and e_r^{--}, $r=1,2,\ldots,(q-1)/2$, those of $\det(m^{--}_{p/q}(e))=0$. And thanks to:

- $\sum_{r=1}^{q}(-1)^r e_r(4)$ happening to rewrite as

$$-\sum_{r=1}^{q}(-1)^r e_r(4) = \sum_{r=1}^{\frac{q+1}{2}}|e_r^{++}| - \sum_{r=1}^{\frac{q-1}{2}}|e_r^{--}|$$

(9) becomes tractable since it reduces to the sum of the absolute values of the roots of two polynomial equations.

Indeed, by using [1]

$$\frac{2\mathrm{i}}{\pi}\int_{-\mathrm{i}x}^{\mathrm{i}x}\left(\frac{z}{z-a}-1\right)\mathrm{d}z=\frac{4a}{\pi}\arctan(\frac{x}{a}),$$

$$\lim_{x\to\infty}\frac{4a}{\pi}\arctan(\frac{x}{a})=2|a|$$

and

$$\lim_{x\to\infty}\frac{2\mathrm{i}}{\pi}\int_{-\mathrm{i}x}^{\mathrm{i}x}\left(\frac{z}{z-a}-1\right)\mathrm{d}z=\lim_{x\to\infty}\frac{2\mathrm{i}}{\pi}\int_{-\mathrm{i}x}^{\mathrm{i}x}\left(-\log\frac{z-a}{z}\right)\mathrm{d}z$$

one gets

$$2\left(\sum_{r=1}^{\frac{q+1}{2}}|e_r^{++}|-\sum_{r=1}^{\frac{q-1}{2}}|e_r^{--}|\right)=\frac{2\mathrm{i}}{\pi}\lim_{x\to\infty}\int_{-\mathrm{i}x}^{\mathrm{i}x}\log\left(\frac{z\det(m_{p/q}^{--}(z))}{\det(m_{p/q}^{++}(z))}\right)\mathrm{d}z. \quad (10)$$

Making [1] further algebraic manipulations on the ratio of determinants in (10), in particular in terms of particular solutions $\{\Phi_0,\Phi_1,\ldots,\Phi_{q-1}\}$ of (2)—on the one hand $\Phi_0=0$ and on the other hand $\Phi_{(q-1)/2}=\Phi_{(q+1)/2}$—and then for large q taking in (1) the continuous limit lead to, via the change of variable $y=qz/(8\pi\mathrm{i})$,

$$\lim_{q\to\infty}2q\left(\sum_{r=1}^{\frac{q+1}{2}}|e_r^{++}|-\sum_{r=1}^{\frac{q-1}{2}}|e_r^{--}|\right)=32\int_0^\infty\log\left(\frac{\Gamma(3/4+y)^2}{y\Gamma(1/4+y)^2}\right)\mathrm{d}y.$$

This last integral gives the first moment

$$\lim_{q\to\infty}q\left(\sum_{r=1}^{q}(-1)^r\big(e_r(-4)-e_r(4)\big)\right)=\frac{4}{\pi}\left(\psi^{(1)}\left(\frac{1}{4}\right)-\pi^2\right) \quad (11)$$

which is a rewriting of (6) ($\psi^{(1)}$ is the polygamma function of order 1).

3. The *n*th moment

3.1. n odd

To evaluate the nth moment one follows the steps above by first noticing in (9) that

$$-\sum_{r=1}^{q}(-1)^r e_r^n(4)=\sum_{r=1}^{\frac{q+1}{2}}|e_r^{++}|^n-\sum_{r=1}^{\frac{q-1}{2}}|e_r^{--}|^n$$

holds. Then using

$$\frac{2\mathrm{i}}{\pi}\int_{-\mathrm{i}x}^{\mathrm{i}x}\left(\frac{z^n}{z-a}-\sum_{k=0}^{n-1}a^k z^{n-1-k}\right)\mathrm{d}z=\frac{4a^n}{\pi}\arctan(\frac{x}{a}),$$

$$\lim_{x\to\infty}\frac{4a^n}{\pi}\arctan(\frac{x}{a})=2|a^n|$$

and

$$\lim_{x\to\infty}\frac{2\mathrm{i}}{\pi}\int_{-\mathrm{i}x}^{\mathrm{i}x}\left(\frac{z^n}{z-a}-\sum_{k=0}^{n-1}a^k z^{n-1-k}\right)\mathrm{d}z=\lim_{x\to\infty}\frac{2\mathrm{i}}{\pi}\int_{-\mathrm{i}x}^{\mathrm{i}x}-nz^{n-1}\left(\log\frac{z-a}{z}+\sum_{k=1}^{n-1}\frac{a^k}{kz^k}\right)\mathrm{d}z \tag{12}$$

one gets

$$2\left(\sum_{r=1}^{\frac{q+1}{2}}|e_r^{++}|^n-\sum_{r=1}^{\frac{q-1}{2}}|e_r^{--}|^n\right)=\frac{2\mathrm{i}}{\pi}\lim_{x\to\infty}\int_{-\mathrm{i}x}^{\mathrm{i}x}nz^{n-1}\left(\log\left(\frac{z\det(m_{p/q}^{--}(z))}{\det(m_{p/q}^{++}(z))}\right)\right.$$
$$\left.-\sum_{k=1}^{n-1}\frac{\sum_{r=1}^{\frac{q+1}{2}}(e_r^{++})^k-\sum_{r=1}^{\frac{q-1}{2}}(e_r^{--})^k}{kz^k}\right)\mathrm{d}z. \tag{13}$$

In the RHS of (12) the polynomial $z^{n-1}\sum_{k=1}^{n-1}\frac{a^k}{kz^k}$ cancels the positive or null exponents in the expansion around $z=\infty$ of the logarithm term $z^{n-1}\log\frac{z-a}{z}$. Likewise, in (13), the same mechanism takes place for $-z^{n-1}\left(\sum_{k=1}^{n-1}\frac{\sum_{r=1}^{\frac{q+1}{2}}(e_r^{++})^k-\sum_{r=1}^{\frac{q-1}{2}}(e_r^{--})^k}{kz^k}\right)$ with respect to $z^{n-1}\log\left(\frac{z\det(m_{p/q}^{--}(z))}{\det(m_{p/q}^{++}(z))}\right)$. Additionally, the polynomials can be reduced to their k even components. Further algebraic manipulations in (13) and, when q is large, taking the continuous limit, lead to, via the change of variable $y=qz/(8\pi\mathrm{i})$,

$$\lim_{q\to\infty}2q^n\left(\sum_{r=1}^{\frac{q+1}{2}}|e_r^{++}|^n-\sum_{r=1}^{\frac{q-1}{2}}|e_r^{--}|^n\right)=(8\pi\mathrm{i})^{n-1}32$$
$$\int_0^\infty ny^{n-1}\left(\log\left(\frac{\Gamma(3/4+y)^2}{y\Gamma(1/4+y)^2}\right)+\sum_{k=2,k\text{ even}}^{n-1}\frac{E_k}{k4^k y^k}\right)\mathrm{d}y. \tag{14}$$

To go from (13) to (14) one has used that for k even, necessarily[2]

$$\lim_{q\to\infty}q^k\left(\sum_{r=1}^{\frac{q+1}{2}}(e_r^{++})^k-\sum_{r=1}^{\frac{q-1}{2}}(e_r^{--})^k\right)=(2\pi)^k|E_k| \tag{15}$$

where the E_k's are the Euler numbers, a result which is also strongly supported by numerical simulations. Indeed in (14), as it was the case in (12,13), the polynomial $\sum_{k=2,k\text{ even}}^{n-1}E_k/(k4^k)y^{n-1-k}$ cancels the positive or null exponents in the expansion around $y=\infty$ of the logarithm term $y^{n-1}\log\left(\frac{\Gamma(3/4+y)^2}{y\Gamma(1/4+y)^2}\right)$—see the appendix for a proof. It amounts to a fine tuning at the infinite upper integration limit so that after integration the end result is finite. Performing this last integral gives the nth moment—see the appendix for details

$$\lim_{q\to\infty}q^n\left(\sum_{r=1}^{q}(-1)^r\left(e_r^n(-4)-e_r^n(4)\right)\right)=\frac{4}{\pi}\left((-1)^{n-1}\psi^{(n)}\left(\frac{1}{4}\right)-2^n\left(2^{n+1}-1\right)\zeta(n+1)n!\right) \tag{16}$$

[2] More generally the kth moments $\sum_{r=1}^{\frac{q+1}{2}}(e_r^{++})^k$ and $\sum_{r=1}^{\frac{q-1}{2}}(e_r^{--})^k$ can be directly retrieved from the coefficients of $\det(m_{p/q}^{++}(e))$ and $\det(m_{p/q}^{--}(e))$, respectively. In particular, one finds $\sum_{r=1}^{\frac{q+1}{2}}e_r^{++}=2$ and $\sum_{r=1}^{\frac{q-1}{2}}e_r^{--}=-2$; for k odd $\lim_{q\to\infty}\sum_{r=1}^{\frac{q+1}{2}}(e_r^{++})^k=4^k/2$ and $\lim_{q\to\infty}\sum_{r=1}^{\frac{q-1}{2}}(e_r^{--})^k=-4^k/2$; for k even $\lim_{q\to\infty}1/q\left(\sum_{r=1}^{\frac{q-1}{2}}(e_r^{++})^k\right)=\lim_{q\to\infty}1/q\left(\sum_{r=1}^{\frac{q-1}{2}}(e_r^{--})^k\right)=\binom{k}{k/2}^2/2$. This last result can easily be understood in terms of the number $\binom{k}{k/2}^2$ of closed lattice walks with k steps [6].

which generalizes the Thouless formula (11) to n odd ($\psi^{(n)}$ is the polygamma function of order n).

3.2. n even

As said above, the nth moment trivially vanishes when n is even. In this case, we should rather consider a nth moment restricted to the positive—or equivalently by symmetry negative—half of the spectrum[3]. In the q odd case it is

$$\begin{aligned} &-\sum_{r=1}^{(q-1)/2}(-1)^r\left(e_r^n(-4)-e_r^n(4)\right)+e^n_{(q+1)/2}\left((-1)^{\frac{q+1}{2}}4\right)\\ &=\sum_{(q+3)/2}^{q}(-1)^r\left(e_r^n(-4)-e_r^n(4)\right)+e^n_{(q+1)/2}\left((-1)^{\frac{q-1}{2}}4\right). \end{aligned} \tag{17}$$

It is still true that

$$\sum_{r=1}^{\frac{q+1}{2}}(e_r^{++})^n-\sum_{r=1}^{\frac{q-1}{2}}(e_r^{--})^n=\sum_{(q+3)/2}^{q}(-1)^r\left(e_r^n(-4)-e_r^n(4)\right)+e^n_{(q+1)/2}\left((-1)^{\frac{q-1}{2}}4\right)$$

where, since n is even, absolute values are not needed anymore, a simpler situation. It follows that the RHS of (16) also gives, when n is even, twice the $q\to\infty$ limit of the half-spectrum nth moment as defined in (17), up to a factor q^n.

3.3. Any n

One reaches the conclusion that

$$\begin{aligned} &\frac{4}{\pi}\left((-1)^{n-1}\psi^{(n)}\left(\frac{1}{4}\right)-2^n\left(2^{n+1}-1\right)\zeta(n+1)n!\right)\\ &=\frac{2}{\pi}4^{n+1}n!\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)^{n+1}}\\ &=\frac{2}{\pi}n!\big(\zeta(n+1,\frac{1}{4})-\zeta(n+1,\frac{3}{4})\big)\\ &=\frac{2}{\pi}(-1)^{n+1}\left(\psi^{(n)}\left(\frac{1}{4}\right)-\psi^{(n)}\left(\frac{3}{4}\right)\right) \end{aligned} \tag{18}$$

yields q^n times the nth moment when n is odd[4]

[3] Instead of $n\int_{-4}^{4}\tilde\rho_{p/q}(e)\mathrm{e}^{n-1}\mathrm{d}e$ one considers

$$n\int_{-4}^{0}\tilde\rho_{p/q}(e)\mathrm{e}^{n-1}\mathrm{d}e=n\int_{0}^{4}\tilde\rho_{p/q}(e)\mathrm{e}^{n-1}\mathrm{d}e.$$

[4] When n is odd it is also twice the half-spectrum nth moment

$$n\int_{-4}^{4}\tilde\rho_{p/q}(e)\mathrm{e}^{n-1}\mathrm{d}e=2n\int_{0}^{4}\tilde\rho_{p/q}(e)\mathrm{e}^{n-1}\mathrm{d}e.$$

and twice the half-spectrum nth moment when n is even. Numerical simulations confirm this result convincingly (even though the convergence is slow when n becomes large). In the n even case one already knows from (15) that (18) simplifies further to

$$2|E_n|\left(2\pi\right)^n$$

from which one gets for the $n\to\infty$-moment scaling

$$\frac{8}{\pi}n!2^{2n}.$$

4. Conclusion and opened issues

(18) is certainly a simple and convincing nth moment generalization of the Thouless bandwidth formula (6). It remains to be proven on more solid grounds for example in the spirit of [5].

In the definition of the nth moment (7), one can view the exponent n as a magnifying loupe of the Thouless first moment. (18) was obtained for $p=1$ (or $q-1$); it would certainly be interesting to understand what happens for $p\neq 1$ where numerical simulations indicate a strong p dependence when n increases, an effect of the n-zooming inherent to the nth moment definition (7).

In the n even case, twice the half-spectrum nth moment ends up being equal to $2|E_n|(2\pi/q)^n$, a result that can be interpreted as if, at the n-zooming level, they were $2|E_n|$ bands each of length $2\pi/q$. It would be interesting to see if this Euler counting has a meaning in the context of lattice walks [6] (twice the Euler number $2|E_n|$ counts the number of alternating permutations in S_n).

Finally, returning to the bandwidth nth moment defined in (8) for n odd, and focusing again on q odd, one can expand

$$\sum_{r=1}^{q}(-1)^r\left(e_r(-4)-e_r(4)\right)^n=-2\sum_{k=0}^{(n-1)/2}\binom{n}{k}(-1)^k\sum_{r=1}^{q}(-1)^r e_r(-4)^k e_r(4)^{n-k} \tag{19}$$

where the symmetry $e_r(-4)=-e_{q+1-r}(4)$ has again been used. The $k=0$ term $-2\sum_{r=1}^{q}(-1)^r e_r(4)^n$ is the nth moment discussed above and one knows that multiplying it by q^n ensures in the $q\to\infty$ limit a finite scaling. Let us also multiply in (19) the $k=1,\ldots,(n-1)/2$ terms by q^n: one checks numerically that

$$\begin{aligned}\lim_{q\to\infty}-2q^n\sum_{r=1}^{q}(-1)^r e_r(-4)^k e_r(4)^{n-k}&=\frac{n-2k}{n}\lim_{q\to\infty}-2q^n\sum_{r=1}^{q}(-1)^r e_r(4)^n\\&=\frac{n-2k}{n}\frac{4}{\pi}\left((-1)^{n-1}\psi^{(n)}\left(\frac{1}{4}\right)-2^n\left(2^{n+1}-1\right)\zeta(n+1)n!\right).\end{aligned}$$

Using

$$\sum_{k=0}^{(n-1)/2}\binom{n}{k}(-1)^k\frac{n-2k}{n}=0$$

one concludes that in the $q\to\infty$ limit the bandwidth nth moment is such that

$$\lim_{q\to\infty} q^n \sum_{r=1}^{q} (-1)^r \big(e_r(-4) - e_r(4)\big)^n = 0$$

when n is odd and larger than 1, a fact which is also supported by numerical simulations. Similarly, when n is even, the bandwidth nth moment, now defined as

$$\sum_{r=1}^{q} \big(e_r(-4) - e_r(4)\big)^n,$$

is such that $\lim_{q\to\infty} q^n \sum_{r=1}^{q} \big(e_r(-4) - e_r(4)\big)^n = 0$.

Clearly, multiplying the sum in (19) by q^n is insufficient, a possible manifestation of the fractal structure [5] of the band spectrum. We leave to further studies the question of finding the right scaling for the bandwidth nth moment.

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Appendix

We want to evaluate the integral (14)

$$I_n = (8\pi \mathrm{i})^{n-1} \cdot 32 \int_0^\infty n y^{n-1} \left(\log\left(\frac{\Gamma(3/4+y)^2}{y\Gamma(1/4+y)^2} \right) + \sum_{k=2,\, k\,\text{even}}^{n-1} \frac{E_k}{k 4^k y^k} \right) \mathrm{d}y$$

for odd integers n. We will see below that $-\sum_{k=2,\, k\,\text{even}}^{\infty} \frac{E_k}{k4^k y^k}$ is indeed the series expansion of $\log\left(\frac{\Gamma(3/4+y)^2}{y\Gamma(1/4+y)^2}\right)$ as $y \to \infty$. So for $y \to 0$, the expression in parentheses is of order y^{1-n} ($\log y$ for $n = 1$), and it is of order y^{-1-n} as $y \to \infty$. We can now apply integration by parts to obtain

$$I_n = -(8\pi \mathrm{i})^{n-1} \cdot 32 \int_0^\infty y^n \left(\frac{2\Gamma'(3/4+y)}{\Gamma(3/4+y)} - \frac{2\Gamma'(1/4+y)}{\Gamma(1/4+y)} - \frac{1}{y} - \sum_{k=2,\, k\,\text{even}}^{n-1} \frac{E_k}{4^k y^{k+1}} \right) \mathrm{d}y.$$

In the following, $\Psi(x) = \Gamma'(x)/\Gamma(x)$ denotes the digamma function. We first show that

$$2\Psi(3/4+y) - 2\Psi(1/4+y) = \frac{2\Gamma'(3/4+y)}{\Gamma(3/4+y)} - \frac{2\Gamma'(1/4+y)}{\Gamma(1/4+y)} = \sum_{k=0,\, k\,\text{even}}^{\infty} \frac{E_k}{4^k y^{k+1}}.$$

To this end, we use the well-known integral representation [7, 5.9.12]

$$\Psi(z) = \int_0^\infty \left(\frac{\mathrm{e}^{-t}}{t} - \frac{\mathrm{e}^{-zt}}{1-\mathrm{e}^{-t}} \right) \mathrm{d}t,$$

which yields

$$\begin{aligned}
2\Psi(3/4+y)-2\Psi(1/4+y) &= 2\int_0^\infty \Big(\frac{\mathrm{e}^{(-1/4-y)t}}{1-\mathrm{e}^{-t}}-\frac{\mathrm{e}^{(-3/4-y)t}}{1-\mathrm{e}^{-t}}\Big)\,\mathrm{d}t\\
&= 2\int_0^\infty \frac{\mathrm{e}^{(1/4-y)t}}{\mathrm{e}^{t/2}+1}\,\mathrm{d}t\\
&= \int_0^\infty \frac{\mathrm{e}^{-yt}}{\cosh(t/4)}\,\mathrm{d}t\\
&= \int_0^\infty \mathrm{e}^{-yt}\sum_{k=0,\,k\,\text{even}}^{\infty}\frac{E_k t^k}{4^k k!}\,\mathrm{d}t\\
&= \sum_{k=0,\,k\,\text{even}}^{\infty}\frac{E_k}{4^k k!}\int_0^\infty t^k\mathrm{e}^{-yt}\,\mathrm{d}t\\
&= \sum_{k=0,\,k\,\text{even}}^{\infty}\frac{E_k}{4^k k!}\cdot\frac{k!}{y^{k+1}}\\
&= \sum_{k=0,\,k\,\text{even}}^{\infty}\frac{E_k}{4^k y^{k+1}},
\end{aligned}$$

as desired. Integration also yields

$$\log\Big(\frac{\Gamma(3/4+y)^2}{y\Gamma(1/4+y)^2}\Big)=-\sum_{k=2,\,k\,\text{even}}^{\infty}\frac{E_k}{k4^k y^k}.$$

Now we consider the Mellin transform of $2(\Psi(3/4+y)-\Psi(1/4+y))$, i.e.

$$F(s)=\int_0^\infty 2(\Psi(3/4+y)-\Psi(1/4+y))y^{s-1}\,\mathrm{d}y.$$

The integral converges for $0<\mathrm{Re}s<1$. Using the same integral representation as before, we find

$$\begin{aligned}
F(s) &= \int_0^\infty y^{s-1}\int_0^\infty \frac{\mathrm{e}^{-yt}}{\cosh(t/4)}\,\mathrm{d}t\,\mathrm{d}y\\
&= \int_0^\infty \frac{1}{\cosh(t/4)}\int_0^\infty y^{s-1}\mathrm{e}^{-yt}\,\mathrm{d}y\,\mathrm{d}t\\
&= \Gamma(s)\int_0^\infty \frac{t^{-s}}{\cosh(t/4)}\\
&= 2\Gamma(s)\int_0^\infty t^{-s}\frac{\mathrm{e}^{-t/4}-\mathrm{e}^{-3t/4}}{1-\mathrm{e}^{-t}}\,\mathrm{d}t.
\end{aligned}$$

Now we use the following integral representation of the Hurwitz zeta function [7, 25.11.25]:

$$\zeta(s,a)=\frac{1}{\Gamma(s)}\int_0^\infty \frac{t^{s-1}\mathrm{e}^{-at}}{1-\mathrm{e}^{-t}}\,\mathrm{d}t$$

for $a>0$ and $\mathrm{Re}s>1$. This gives us

$$\zeta(s,1/4)-\zeta(s,3/4)=\frac{1}{\Gamma(s)}\int_0^\infty \frac{t^{s-1}(\mathrm{e}^{-t/4}-\mathrm{e}^{-3t/4})}{1-\mathrm{e}^{-t}}\,\mathrm{d}t,$$

a priori only for $\mathrm{Re}s > 1$. However, the integral also converges for $\mathrm{Re}s > 0$, so the identity remains true by analytic continuation. Hence we have

$$F(s) = 2\Gamma(s)\Gamma(1-s)(\zeta(1-s,1/4) - \zeta(1-s,3/4)).$$

The functional equations of the Gamma function and the Hurwitz zeta function yield

$$\Gamma(s)\Gamma(1-s) = \frac{\pi}{\sin(\pi s)}$$

and

$$\zeta(1-s,1/4) - \zeta(1-s,3/4) = \frac{4\Gamma(s)\sin(\pi s/2)}{(8\pi)^s}\big(\zeta(s,1/4) - \zeta(s,3/4)\big),$$

so

$$F(s) = \frac{4\pi\Gamma(s)}{(8\pi)^s\cos(\pi s/2)}\big(\zeta(s,1/4) - \zeta(s,3/4)\big).$$

Now we use the general property of the Mellin transform (see [8, p 19]) that subtracting off terms of the asymptotic expansion at either 0 or ∞ only changes the fundamental strip of the Mellin transform, but not the transform itself. Thus we have

$$\begin{aligned} I_n &= -(8\pi\mathrm{i})^{n-1}\cdot 32\cdot\frac{4\pi\Gamma(n+1)}{(8\pi)^{n+1}\cos(\pi(n+1)/2)}\big(\zeta(n+1,1/4) - \zeta(n+1,3/4)\big) \\ &= \frac{2}{\pi}n!\big(\zeta(n+1,1/4) - \zeta(n+1,3/4)\big) \end{aligned}$$

which is (16) and (18).

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Chapter

5 Epilogue

In this epilogue, we highlight the main results obtained above and the new questions raised by them. We give a brief discussion on the perspectives of the results obtained from this work and the further works to be done.

The main subject of this thesis is the deep connection between the Hofstadter model and planar random lattice walks. In chapter 1, we introduced $Z_n(Q)$, the algebraic area generating function of closed random walks of length n on a $2d$ lattice, and discussed the formal mapping between $\mathsf{Tr}H_\gamma^n$, the n-th moment of the Hofstadter Hamiltonian (where γ denote the ratio between the magnetic flux through a unit cell of the lattice and the flux quantum) and $Z_n(e^{i\gamma})$, namely $\mathsf{Tr}H_\gamma^n = Z_n(e^{i\gamma})$. We were interested in the case where $e^{i\gamma}$ is a root of unity ("rational case" i.e. $\gamma = 2\pi p/q$ with p and q are coprime integers). In chapter 2, from the random walk approach, we found the explicit formula for $Z_n(e^{2\pi i p/q})$ in eq. (2.23) in terms of the Kreft coefficients $a_{p/q}(2j)$ defined in eq. (2.18). They are the coefficients of the characteristic polynomial $E^q b_{p/q}(1/E)$ eq. (3.7) of degree q encoding the wave number independent part of the determinant of the Hofstadter's Hamiltonian eq. (3.2). More importantly, a closed expression for $C_n(A)$, the number of closed random walks of length n enclosing a given algebraic area A remains an open issue. We made recent progress indicating that this type of information is contained in the Kreft coefficients $a_{p/q}(2j)$ given in eq. (2.18). These coefficients are clearly defined for $q > 2j$. An open related question is how to generalize them to any value of q. With the Mathematica Simplify command acting on eq. (2.18), one can find expression for $a_{p/q}(2j)$ trigonometric. For examples when $2j = 2, 4, 6$:

$$
\begin{aligned}
a_{p/q}(2) &= 2q \\
a_{p/q}(4) &= q\left(7 + 2\cos\left(\frac{2\pi p}{q}\right) - 2q\right) \\
a_{p/q}(6) &= \frac{2q}{3}\left(58 + 36\cos\left(\frac{2\pi p}{q}\right) + 6\cos\left(\frac{4\pi p}{q}\right) - q\left(21 + 6\cos\left(\frac{2\pi p}{q}\right)\right) + 2q^2\right)
\end{aligned}
$$

As the above examples indicate, $a_{p/q}(2j)$ can be rewritten as a polynomial of q with maximal degree j. By computing the part of $a_{p/q}(2j)$ linear in q, its $\cos\left(\frac{2k\pi p}{q}\right)$ expansion gives the number of closed random walks of length $2j$ with the algebraic area $\pm k$ ($+$ when random walks move in counterclockwise, otherwise $-$). Therefore, finding a way to rewrite the Kreft coefficients $a_{p/q}(2j)$ and compute their order q part can give us a closed expression for the number of closed random walks of a given length enclosing a given algebraic area [29].

In chapter 3, we introduced the point spectrum trace $\sum_{r=1}^{q} E_r(s)^n$ eq. (3.15) as a tool to recover the Hofstadter trace by integrating it with the suitable density of the state $\rho(s)$ eq. (3.18). The explicit formula of the point trace $\mathrm{Tr}_{\pm\mathrm{s}} H^n_{2\pi p/q}$ is given in eq. (3.15). The method we used for the Hofstadter model is generalized for the almost Mathieu operator section 3.3. We have noticed that as soon as $q > n/2$, the expression $\sum_{r=1}^{q} E_r^n(s)$ does not depend on s anymore. In the limit q goes to infinity (zero magnetic flux), $\sum_{r=1}^{q} E_r(s)^n = \binom{n}{n/2}^2$ (it can easily be understood as the number of closed random walks with n even steps). Numerical simulations also indicate that $\sum_{r=1}^{q} |E_r(s)|^n = \binom{n}{n/2}^2$ when n is odd. It turns out this last result can be explicitly derived. We are looking at finding an analytical expression of $\sum_{r=1}^{q} |E_r(s)|^n$ for a finite q. This quantity may be related to graph theory, because the

energy of a graph [30] is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. This concept is intimately related to the Hückel molecular orbital theory (which is called the tight binding method in solid-state physics and the Hofstadter model is a $2d$ tight binding model subjected to a perpendicular magnetic field). In this context, a graph is used to represent a molecule by considering the atoms as the vertices of the graph and the molecular bonds as the edges, so we have a direct map between a molecule and a graph. Therefore their eigenvalues are simply related to each other [31].

In chapter 4, still in the "rational case", for a given magnetic flux $\gamma = 2\pi p/q$, there are q energy bands. For q odd, $(-1)^r \left(E_r(-4) - E_r(4)\right)$ is the bandwidth of the r-th band $(r = 1, 2, \ldots, q)$ where $E_r(4)$ and $E_r(-4)$ are the two edges of the r-th band. When n is odd, the n-th moment bandwidth is defined as in eq. (4.2)

$$\sum_{r=1}^{q} (-1)^r \left(E_r(-4) - E_r(4)\right)^n$$

We are interested in finding the appropriate scaling for this n-th moment in the limit q goes to infinity. In [20], Thouless found that for $n = 1$ the bandwidth multiplied by q scales like $32\ G/\pi$, where $G = \sum_{k=0}^{\infty} (-1)^k \frac{1}{(2k+1)^2}$ is the Catalan constant. By using Thouless method, in chapter 4, we were able to generalize the Thouless bandwidth formula to a truncated n-th moment bandwidth, namely $\sum_{i=1}^{q} (-1)^r \left(E_r^n(-4) - E_r^n(4)\right)$. In the limit q goes to infinity, when multiplied by q^n, it scales like $\frac{2}{\pi} 4^{n+1} n! \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^{n+1}}$, eq. (4.16) (this is the Dirichlet beta function $\beta(n+1)$ also known as the Catalan beta function). The actual scaling of the n-th moment bandwidth remains an open issue. It should be remarked that numerical simulations indicate that there might exist a multifractal structure at work. Meanwhile, we know that in the case γ being irrational, the spectrum of the Hofstadter model is a Cantor set (i.e. a nowhere dense set and has no isolated point [5]). Hence, the difference between the case γ rational and irrational remains to be discussed in more details and finding the right scaling of the n-th moment bandwidth would be interesting in this regard.

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Appendix

A Kreft's coefficients construction

Following Kreft [15] we show how to get a closed expression for the polynomial (3.26), i.e. for the Kreft coefficients $a^{(\lambda)}_{p/q}(2j)$ in $b^{(\lambda)}_{p/q}(z) = -\sum_{j=0}^{[\frac{q}{2}]} a^{(\lambda)}_{p/q}(2j) z^{2j}$ as defined in (3.24).

$\lambda = 2$**:**

One aims at transforming the matrix $m_{p/q}(E, k_x, k_y)$ in (3.3) into a tridiagonal one by an appropriate change of basis. First, let us do the change of basis

$$m_1 = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & e^{ik_x} & 0 & \cdots & 0 & 0 \\ 0 & 0 & e^{i2k_x} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & e^{i(q-2)k_x} & 0 \\ 0 & 0 & 0 & \cdots & 0 & e^{i(q-1)k_x} \end{pmatrix}$$

so that $m_{p/q}(E, k_x, k_y)$ rewrites as

$$m_1^{-1} m_{p/q}(E, k_x, k_y)\, m_1 = \begin{pmatrix} 2\cos(k_y) - E & e^{ik_x} & 0 & \cdots & 0 & e^{-ik_x} \\ e^{-ik_x} & 2\cos\left(k_y + \frac{2\pi p}{q}\right) - E & e^{ik_x} & \cdots & 0 & 0 \\ 0 & e^{-ik_x} & () & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & () & e^{ik_x} \\ e^{ik_x} & 0 & 0 & \cdots & e^{-ik_x} & 2\cos\left(k_y + (q-1)\frac{2\pi p}{q}\right) - E \end{pmatrix}$$

In this new basis the Schrödinger equation (**??**) with $\Phi_{m+q} = e^{iqk_x}\Phi_m$ becomes

$$e^{ik_x}\Phi'_{m+1} + e^{-ik_x}\Phi'_{m-1} + 2\cos(k_y + \gamma m)\,\Phi'_m = E\Phi'_m, \quad \Phi'_{m+q} = \Phi'_m$$

Then let us do a second change of basis m_2 with matrix element

$$m_{jk} = \frac{1}{\sqrt{q}}(-1)^{pk} e^{\frac{2i\pi p}{q}(jk - k^2/2)}, \quad k, j \in \{0, 1, \ldots, q-1\}.$$

Putting together m_1 and m_2 amounts to the change of basis $m_1 m_2$ with matrix element $e^{ikk_x} m_{jk} = e^{ikk_x} \frac{1}{\sqrt{q}}(-1)^{pk} e^{\frac{2i\pi p}{q}(jk - k^2/2)}$

$$(m_1 m_2)^{-1} m_{p/q}(E, k_x, k_y)\, m_1 m_2 = \begin{pmatrix} -E & \alpha_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}_{p/q}(q-1) \\ \overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-2) \\ \alpha_{p/q}(q-1) & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-2) & -E \end{pmatrix} \tag{A.1}$$

where $\alpha_{p/q}(k) = e^{-ik_y} - (-1)^{(p+1)} e^{\frac{2i\pi p}{q}(k+1/2)+ik_x}$, $\overline{\alpha}_{p/q}(k)$ is its complex conjugate and accordingly

$$\alpha_{p/q}(m)\tilde{\Phi}_{m+1} + \overline{\alpha}_{p/q}(m-1)\tilde{\Phi}_{m-1} = E\tilde{\Phi}_m, \quad \tilde{\Phi}_{m+q} = \tilde{\Phi}_m \tag{A.2}$$

Both corners $\alpha_{p/q}(q-1)$ and $\overline{\alpha}_{p/q}(q-1)$ in the matrix (A.1) can be cancelled if $e^{i(k_x+k_y)} = (-1)^{(p+1)} e^{-\frac{2i\pi p}{q}(q-1+1/2)} = (-1)^{(p+1)} e^{\frac{i\pi p}{q}}$, i.e. if $k_x+k_y = \pi(p+1)+\frac{\pi p}{q}$. The matrix is then tridiagonal with a determinant in (**??**) equal to $(-1)^q E^q b_{p/q}(1/E)$, since the trigonometric part vanishes as well: indeed

$$\begin{aligned}
\cos(qk_x) + \cos(qk_y) &= 2\cos\left(\frac{q(k_x+k_y)}{2}\right)\cos\left(\frac{q(k_x-k_y)}{2}\right) \\
&= 2\cos\left(\frac{\pi(p+q(p+1))}{2}\right)\cos\left(\frac{q(k_x-k_y)}{2}\right) \\
&= 0
\end{aligned}$$

due to $p+q(p+1)$ being always odd since p and q are co-prime.

One gets the tridiagonal matrix

$$\begin{pmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0 \\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-2) \\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-2) & -E
\end{pmatrix} \tag{A.3}$$

where $\alpha_{p/q}(k)$, using $e^{i(k_x+k_y)} = (-1)^{(p+1)} e^{\frac{i\pi p}{q}}$, has simplified to $\alpha_{p/q}(k) = e^{-ik_y}(1 - e^{\frac{2i\pi(k+1)p}{q}})$. The matrix (A.3) does not depend anymore on k_x nor k_y and its determinant satisfies a recursion (see [15]) leading respectively to the Kreft polynomial (**??**)and Kreft coefficients (**??**).

$\lambda \neq 2$:

One uses the same method as above to find a closed expression for the polynomial $b^{(\lambda)}_{p/q}(1/E)$, namely transform the matrix $m^{(\lambda)}_{p/q}(E, k_x, k_y)$ in (3.21) into a tridiagonal one. To do so use the same change of basis $m_1 m_2$ as above so that

$$(m_1 m_2)^{-1} m^{(\lambda)}_{p/q}(E, k_x, k_y,)\, m_1 m_2 = \begin{pmatrix}
-E & \alpha^{(\lambda)}_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}^{(\lambda)}_{p/q}(q-1) \\
\overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\
\alpha^{(\lambda)}_{p/q}(q-1) & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E
\end{pmatrix} \tag{A.4}$$

with $\alpha^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{-ik_y} - (-1)^{p+1} e^{i\frac{2\pi p}{q}(k+1/2)+ik_x}$ and $\overline{\alpha}^{(\lambda)}_{p/q}(k)$ its complex conjugate. Moreover, we have a resulting Schrödinger equation identical to (A.2) provided that $\alpha_{p/q}(k)$ is replaced with $\alpha^{(\lambda)}_{p/q}(k)$.

Contrary to the Hofstadter case $\lambda = 2$, both corners $\alpha^{(\lambda)}_{p/q}(q-1)$ and $\overline{\alpha}^{(\lambda)}_{p/q}(q-1)$ in the matrix (A.4) cannot simultaneously vanish. One can still choose to have the lower left corner $\alpha^{(\lambda)}_{p/q}(q-1)$ to vanish: this amounts to $e^{i(k_x+k_y)} = (-1)^{p+1}(\lambda/2)e^{-i\frac{2\pi p}{q}(q-1+1/2)} = (-1)^{p+1}(\lambda/2)e^{\frac{i\pi p}{q}}$, which can only be achieved for a complex $k_x + k_y$ (namely $k_x + k_y = -i\log(\lambda/2) + \frac{\pi p}{q} + \pi(p+1)$), so that

$e^{-i(k_x+k_y)} = (-1)^{p+1}(2/\lambda)e^{-\frac{i\pi p}{q}}$. The matrix (A.4) then becomes

$$\begin{pmatrix} -E & \alpha^{(\lambda)}_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}^{(\lambda)}_{p/q}(q-1) \\ \overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\ 0 & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E \end{pmatrix} \tag{A.5}$$

where $\alpha^{(\lambda)}_{p/q}(k)$ and $\overline{\alpha}^{(\lambda)}_{p/q}(k)$ have simplified to $\alpha^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{-ik_y}(1 - e^{\frac{2i\pi(k+1)p}{q}})$ and $\overline{\alpha}^{(\lambda)}_{p/q}(k) = (\lambda/2)e^{ik_y}(1 - (2/\lambda)^2 e^{-\frac{2i\pi(k+1)p}{q}})$. Note that $\overline{\alpha}^{(\lambda)}_{p/q}(k)$ is not anymore the complex conjugate of $\alpha^{(\lambda)}_{p/q}(k)$.

By expanding the determinant of (A.5) with respect to the elements of the first row

$$\begin{vmatrix} -E & \alpha^{(\lambda)}_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}^{(\lambda)}_{p/q}(q-1) \\ \overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\ 0 & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E \end{vmatrix} = -E \begin{vmatrix} -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\ \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\ 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E \end{vmatrix}$$

$$- \alpha^{(\lambda)}_{p/q}(0)\overline{\alpha}^{(\lambda)}_{p/q}(0) \begin{vmatrix} -E & \alpha^{(\lambda)}_{p/q}(2) & \cdots & 0 & 0 \\ \overline{\alpha}^{(\lambda)}_{p/q}(2) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\ 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E \end{vmatrix}$$

$$+ (-1)^{q+1}\overline{\alpha}^{(\lambda)}_{p/q}(q-1) \begin{vmatrix} \overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-3) & -E \\ 0 & 0 & 0 & \cdots & 0 & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) \end{vmatrix} \tag{A.6}$$

it is immediate to see that the part that depends on k_x or k_y can only come from the last term of (A.6), i.e. from the upper right corner $\overline{\alpha}^{(\lambda)}_{p/q}(q-1)$. Therefore to get the desired k_x, k_y-independent polynomial $E^q b^{(\lambda)}_{p/q}(1/E)$, all that is needed is the determinant of the tridiagonal matrix

$$\begin{pmatrix} -E & \alpha^{(\lambda)}_{p/q}(0) & 0 & \cdots & 0 & 0 \\ \overline{\alpha}^{(\lambda)}_{p/q}(0) & -E & \alpha^{(\lambda)}_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}^{(\lambda)}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha^{(\lambda)}_{p/q}(q-2) \\ 0 & 0 & 0 & \cdots & \overline{\alpha}^{(\lambda)}_{p/q}(q-2) & -E \end{pmatrix}$$

which finally yields the $\lambda \neq 2$ Kreft polynomial (3.26) and Kreft coefficients (3.25).

Appendix

B Chamber's identity

With the change of basis eq. (A.1) it is easy to identify the trigonometric part $2(\cos(qk_x)+\cos(qk_y))$ in Chambers's identity eq. (3.6) as $\prod_{k=0}^{q-1}\alpha_{p/q}(k)+\prod_{k=0}^{q-1}\overline{\alpha}_{p/q}(k)$; one can also verify $\sum_{k=0}^{q-1}\alpha_{p/q}(k)\overline{\alpha}_{p/q}(k) = a_{p/q}(2) = 2q$.

Indeed by expanding the determinant of eq. (A.1) with respect to its last column

$$
\begin{vmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}_{p/q}(q-1) \\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-2) \\
\alpha_{p/q}(q-1) & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-2) & -E
\end{vmatrix} =
$$

$$
(-1)^{q+1}\overline{\alpha}_{p/q}(q-1)
\begin{vmatrix}
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\
0 & 0 & \overline{\alpha}_{p/q}(2) & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-3) & -E \\
\alpha_{p/q}(q-1) & 0 & 0 & \cdots & 0 & \overline{\alpha}_{p/q}(q-2)
\end{vmatrix}
$$

$$
-\alpha_{p/q}(q-2)
\begin{vmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0 \\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-3) \\
\alpha_{p/q}(q-1) & 0 & 0 & \cdots & 0 & \overline{\alpha}_{p/q}(q-2)
\end{vmatrix}
$$

$$
-e
\begin{vmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0 \\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-3) \\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-3) & -E
\end{vmatrix}
$$

and then by expanding the first two determinants with respect to their last row one gets

$$
\begin{aligned}
&-\alpha_{p/q}(q-1)\overline{\alpha}_{p/q}(q-1)\begin{vmatrix}
-E & \alpha_{p/q}(1) & 0 & \cdots & 0 & 0\\
\overline{\alpha}_{p/q}(1) & -E & \alpha_{p/q}(2) & \cdots & 0 & 0\\
0 & \overline{\alpha}_{p/q}(2) & -E & \cdots & 0 & 0\\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-3)\\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-3) & -E
\end{vmatrix}\\
&+(-1)^{q+1}\overline{\alpha}_{p/q}(q-1)\,\overline{\alpha}_{p/q}(q-2)\begin{vmatrix}
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0\\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0\\
0 & 0 & \overline{\alpha}_{p/q}(2) & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-4) & -E\\
0 & 0 & 0 & \cdots & 0 & \overline{\alpha}_{p/q}(q-3)
\end{vmatrix}\\
&+(-1)^{q+1}\alpha_{p/q}(q-2)\alpha_{p/q}(q-1)\begin{vmatrix}
\alpha_{p/q}(0) & 0 & 0 & \cdots & 0 & 0\\
-E & \alpha_{p/q}(1) & 0 & \cdots & 0 & 0\\
\overline{\alpha}_{p/q}(1) & -E & \alpha_{p/q}(2) & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & \alpha_{p/q}(q-4) & 0\\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-3)
\end{vmatrix}\\
&-\alpha_{p/q}(q-2)\overline{\alpha}_{p/q}(q-2)\begin{vmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0\\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0\\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-4)\\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-4) & -E
\end{vmatrix}\\
&-E\begin{vmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0\\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0\\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-3)\\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-3) & -E
\end{vmatrix}
\end{aligned}
$$

Both triangular determinants are the product of their diagonal entries, so one gets

$$
\begin{aligned}
&(-1)^{q+1}\prod_{k=0}^{q-1}\overline{\alpha}_{p/q}(k)+(-1)^{q+1}\prod_{k=0}^{q-1}\alpha_{p/q}(k)\\
&-\alpha_{p/q}(q-1)\overline{\alpha}_{p/q}(q-1)\begin{vmatrix}
-E & \alpha_{p/q}(1) & 0 & \cdots & 0 & 0\\
\overline{\alpha}_{p/q}(1) & -E & \alpha_{p/q}(2) & \cdots & 0 & 0\\
0 & \overline{\alpha}_{p/q}(2) & -E & \cdots & 0 & 0\\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-3)\\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-3) & -E
\end{vmatrix}\\
&-\alpha_{p/q}(q-2)\overline{\alpha}_{p/q}(q-2)\begin{vmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0\\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0\\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-4)\\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-4) & -E
\end{vmatrix}\\
&-E\begin{vmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0\\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0\\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-3)\\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-3) & -E
\end{vmatrix}
\end{aligned}
$$

Noticing that the determinant of the $q\times q$ tridiagonal matrix

$$
D_q=\begin{vmatrix}
-E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0\\
\overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0\\
0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-2)\\
0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-2) & -E
\end{vmatrix}
$$

obeys the recursion $D_q=-ED_{q-1}-\alpha_{p/q}(q-2)\overline{\alpha}_{p/q}(q-2)D_{q-2}$ the last two terms can be regrouped

to finally get

$$\begin{vmatrix} -E & \alpha_{p/q}(0) & 0 & \cdots & 0 & \overline{\alpha}_{p/q}(q-1) \\ \overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-2) \\ \alpha_{p/q}(q-1) & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-2) & -E \end{vmatrix} = (-1)^{q+1}\left(\prod_{k=0}^{q-1}\alpha_{p/q}(k) + \prod_{k=0}^{q-1}\overline{\alpha}_{p/q}(k)\right)$$

$$-\alpha_{p/q}(q-1)\overline{\alpha}_{p/q}(q-1)\begin{vmatrix} -E & \alpha_{p/q}(1) & 0 & \cdots & 0 & 0 \\ \overline{\alpha}_{p/q}(1) & -E & \alpha_{p/q}(2) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}_{p/q}(2) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-3) \\ 0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-3) & -E \end{vmatrix}$$

$$+\begin{vmatrix} -E & \alpha_{p/q}(0) & 0 & \cdots & 0 & 0 \\ \overline{\alpha}_{p/q}(0) & -E & \alpha_{p/q}(1) & \cdots & 0 & 0 \\ 0 & \overline{\alpha}_{p/q}(1) & -E & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -E & \alpha_{p/q}(q-2) \\ 0 & 0 & 0 & \cdots & \overline{\alpha}_{p/q}(q-2) & -E \end{vmatrix}$$

where the part $\prod_{k=0}^{q-1}\alpha_{p/q}(k) + \prod_{k=0}^{q-1}\overline{\alpha}_{p/q}(k)$ has been isolated. Now the product $\prod_{k=0}^{q-1}\alpha_{p/q}(k)$ can be rewritten as a polynomial in e^{-ik_y} of degree q

$$\prod_{k=0}^{q-1}\alpha_{p/q}(k) = \prod_{k=0}^{q-1}\left(e^{-ik_y} - (-1)^{p+1}e^{\frac{2i\pi p}{q}(k+1/2)}e^{ik_x}\right) = c_0 + c_1e^{-ik_y} + c_2e^{-i2k_y} + \ldots + c_qe^{-iqk_y}$$

Clearly $c_0 = (-1)^{pq}e^{iqk_x}\prod_{k=0}^{q-1}e^{\frac{2i\pi p}{q}(k+1/2)} = (-1)^{pq}e^{iqk_x}(-1)^{pq} = e^{iqk_x}$ and $c_q = 1$. Assuming now $q > 1$, there are $q-1$ ways to build c_{q-1} at order $e^{-i(q-1)k_y}$, each multiplied by $(-1)^pe^{\frac{2i\pi p}{q}(k+1/2)}e^{ik_x}$

$$c_{q-1} = \sum_{k=0}^{q-1}(-1)^pe^{\frac{2i\pi p}{q}(k+1/2)}e^{ik_x} = (-1)^pe^{i(\frac{\pi p}{q}+k_x)}\sum_{k=0}^{q-1}e^{\frac{2i\pi kp}{q}} = 0$$

since $\sum_{k=0}^{q-1}e^{\frac{2i\pi p}{q}k}$ when $q > 1$, vanishes being the sum of the q-th roots of unity. Likewise assuming $q > 2$ one has for c_{q-2}

$$\begin{aligned} c_{q-2} &= \left((-1)^pe^{i(\frac{\pi p}{q}+k_x)}\right)^2\sum_{k_1=0}^{q-1}\sum_{k_2=k_1+1}^{q-1}e^{\frac{2i\pi(k_1+k_2)p}{q}} \\ &= \left((-1)^pe^{i(\frac{\pi p}{q}+k_x)}\right)^2\sum_{k_1=0}^{q-1}\left(\sum_{k_2=0}^{q-1}e^{\frac{2i\pi(k_1+k_2)p}{q}} - \sum_{k_2=0}^{k_1-1}e^{\frac{2i\pi(k_1+k_2)p}{q}} - e^{\frac{2i\pi k_1p}{q}2}\right) \\ &= \left((-1)^pe^{i(\frac{\pi p}{q}+k_x)}\right)^2\frac{1}{2}\left(\left(\sum_{k=0}^{q-1}e^{\frac{2i\pi kp}{q}}\right)^2 - \sum_{k=0}^{q-1}e^{\frac{2i\pi kp}{q}2}\right) \\ &= 0 \end{aligned}$$

since both $\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}}$ and $\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}2}$ vanish when $q > 2$.
In general using $\sum_{k_1=0}^{q-1}\sum_{k_2=k_1+1}^{q-1} e^{\frac{2i\pi(k_1+k_2)p}{q}} = \frac{1}{2}\left(\sum_{k_1=0}^{q-1}\sum_{k_2=0}^{q-1} e^{\frac{2i\pi(k_1+k_2)p}{q}} - \sum_{k_1=0}^{q-1} e^{\frac{2i\pi k_1 p}{q}2}\right)$, c_{q-j} can be written as

$$\begin{aligned}
c_{q-j} &= \sum_{k_1=0}^{q-1}\sum_{k_2=k_1+1}^{q-1}\cdots\sum_{k_j=k_{j-1}+1}^{q-1}(-1)^{pj}e^{\frac{2i\pi(k_1+k_2+\ldots+k_j+j/2)p}{q}}e^{ijk_x} \\
&= \left((-1)^p e^{i(\frac{\pi p}{q}+k_x)}\right)^j \sum_{k_1=0}^{q-1}\sum_{k_2=k_1+1}^{q-1}\cdots\sum_{k_j=k_{j-1}+1}^{q-1} e^{\frac{2i\pi(k_1+k_2+\ldots+k_j)p}{q}} \\
&= \left((-1)^p e^{i(\frac{\pi p}{q}+k_x)}\right)^j \left(\frac{1}{2}\right)^{j-1} \\
&\left(\left(\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}}\right)^j - (j-1)\left(\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}}\right)^{j-2}\left(\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}2}\right) + \ldots + (-1)^{j-1}\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}j}\right) \\
&= 0
\end{aligned}$$

since $\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}}$, $\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}2} = 0$, … and $\sum_{k=0}^{q-1} e^{\frac{2i\pi kp}{q}j}$ all vanish when $q > j$. Finally

$$\prod_{k=0}^{q-1}\alpha_{p/q}(k) = c_0 + c_q e^{-iqk_y} = e^{iqk_x} + e^{-iqk_y}$$

so that

$$\prod_{k=0}^{q-1}\alpha_{p/q}(k) + \prod_{k=0}^{q-1}\overline{\alpha}_{p/q}(k) = 2\left(\cos(qk_x) + \cos(qk_y)\right)$$

Likewise when $\lambda \neq 2$ it is possible to identify in eq. (3.22) the trigonometric part $2(\cos(qk_x) + (\frac{\lambda}{2})^2\cos(qk_y))$ as $\prod_{k=0}^{q-1}\alpha_{p/q}^{(\lambda)}(k) + \prod_{k=0}^{q-1}\overline{\alpha}_{p/q}^{(\lambda)}(k)$; also one can check $\sum_{k=0}^{q-1}\alpha_{p/q}^{(\lambda)}(k)\overline{\alpha}_{p/q}^{(\lambda)}(k) = a_{p/q}^{(\lambda)}(2) = q + q(\frac{\lambda}{2})^2$.

Appendix

C Energy interval

$\lambda = 2$

In this section, we show eigenenergies of the Harper's equation vary between $[-4, 4]$.

Recall the Harper's equation:

$$\Phi_{m+1} + \Phi_{m-1} + 2\cos(k_y + \gamma m)\phi_m = E\Phi_m \tag{C.1}$$

with $\gamma = 2\pi p/q$. we introduce a new function $t_m = \Phi_m/\Phi_{m-1}$, (C.1) becomes :

$$t_{m+1} = E - 2\cos(k_y + \gamma m) - \frac{1}{t_m} \tag{C.2}$$

$$t_m = \left[E - 2\cos(k_y + \gamma m) - \frac{1}{t_m}\right]^{-1} \tag{C.3}$$

if $|E| \geq E$, we define $|E| = 4 + x$ with $x \geq 0$ and give t_m a initial condition $t_0 = \varrho \exp[i\tau]$ with $\varrho > 0$. Using relations (C.2) and (C.3), we get:

$$t_1 = E - 2\cos(k_y) - \frac{1}{t_0} = E - 2\cos(k_y) - \frac{1}{\varrho \exp[i\tau]}$$

if $\varrho \geq 1$:

$$\begin{aligned}
&t_1 \geq E - 2 - 1 = 4 + x - 3 = 1 + x \\
&t_2 = E - 2\cos(k_y + \gamma) - \frac{1}{t_1} \geq E - 2 - \frac{1}{1+x} \geq E - 3 = 1 + x \\
&\vdots \\
&t_{m+1} = E - 2\cos(k_y + \gamma m) - \frac{1}{t_m} \geq 1 + x
\end{aligned} \tag{C.4}$$

if $\varrho \leq 1$:

$$\begin{aligned}
&t_{-1} = [E - 2\cos(k_y - \gamma) - t_0]^{-1} = [E - 2\cos(k_y - \gamma) - \varrho \exp[i\tau]]^{-1} \\
&t_{-1} \leq [E - 2 - 1]^{-1} = [E - 3]^{-1} = [1 + x]^{-1} \\
&t_{-2} = [E - 2\cos(k_y - 2\gamma) - t_{-1}]^{-1} \leq \left[E - 2 - \frac{1}{x+1}\right]^{-1} \leq [E - 2 - 1]^{-1} = [1 + x]^{-1} \\
&\vdots \\
&t_{-m} = [E - 2\cos(k_y - \gamma m) - t_{-m+1}]^{-1} \leq [1 + x]^{-1}
\end{aligned} \tag{C.5}$$

In the limit $N \to \infty$, from equations (C.4) and (C.5), we get :

$$|t_N t_{N-1} \cdots t_1 t_0| = \left|\frac{\Phi_N}{\Phi_0} \varrho \exp[i\tau]\right| \geq (1 + x)^N \to \infty \tag{C.6}$$

$$|t_{-N}t_{-N+1}\cdots t_{-1}t_0| = \left|\frac{\Phi_0}{\Phi_{-(N+1)}}\right| \leq (1+x)^{-1} \to 0 \tag{C.7}$$

So if $\varrho \geq 1$, $\Phi_{|N|} \to \infty$ and $\Phi_{-|N|} \to \infty$, if $\varrho \leq 1$. Thus $|E| \geq 4$, Φ_m goes to infinity when $m \to \infty$. Consequently $|E|$ must be less then 4 to keep all Φ_m finite.

$\lambda \neq 2$

In this section, we show eigenenergies of the almost Mathieu Operator: $|E^{(\lambda)}| \leq \lambda + 2$

Recall the almost Mathieu Operator (with $\lambda \geq 0$):

$$[H_\theta^{\lambda,\alpha}u](n) = u(n+1) + u(n-1) + \lambda\cos(2\pi\alpha n + \theta)u(n) \tag{C.8}$$

Harper equation (C.1) is just the special case of (C.8) when $\lambda = 2$. Replacing 2 by λ, (C.1) becomes :

$$\Phi_{m+1} + \Phi_{m-1} + \lambda\cos(k_y + \gamma m)\Phi_m = E^{(\lambda)}\Phi_m$$

Using the same method, equations (C.4) and (C.5) become :

$$t_{m+1} = E^{(\lambda)} - \lambda\cos(ky + \gamma m) - \frac{1}{t_m} \geq E^{(\lambda)} - \lambda - 1 \tag{C.9}$$

$$t_m = \Big[E^{(\lambda)} - \lambda\cos(ky + \gamma m) - t_{m+1}\Big]^{-1} \leq \Big[E^{(\lambda)} - \lambda - 1\Big]^{-1} \tag{C.10}$$

(C.6) and (C.7) become :

$$|t_N t_{N-1}\cdots t_1 t_0| = \left|\frac{\Phi_N}{\Phi_0}\varrho\exp[i\tau]\right| \geq (E^{(\lambda)} - \lambda - 1)^N \tag{C.11}$$

$$|t_{-N}t_{-N+1}\cdots t_{-1}t_0| = \left|\frac{\Phi_0}{\Phi_{-(N+1)}}\right| \leq (E^{(\lambda)} - \lambda - 1)^{-1} \tag{C.12}$$

So, to keep all Φ_m finite, $|E^{(\lambda)} - \lambda - 1|$ must less than 1, i.e $|E^{(\lambda)}| \leq \lambda + 2$ is a necessary condition for (C.8).

Appendix

D Simple examples of $Z_{m_1,m_2,l_1,l_2}\left(\exp(2i\pi/q)\right)$

Explicite derivation of $Z_{m_1,m_2,l_1,l_2}\left(\exp(2i\pi/q)\right)$ in the case where $m_1 - m_2 \equiv l_1 - l_2 \equiv 0 \bmod q$ with $q = 2$, $q = 3$ and $q = 4$.

Recall eq. (2.9)

$$A(x_1, x_2, y_1, y_2, Q) = \sum_{m_1,m_2,l_1,l_2 \geq 0} Z_{m_1,m_2,l_1,l_2}(Q) x_1^{m_1} x_2^{m_2} y_1^{l_1} y_2^{l_2}$$

and Cramer's rule :

$$A_0 = A_q = A(x_1, x_2, y_1, y_2, \exp(2i\pi/q)) = \frac{\begin{vmatrix} 1 & -x_2 & 0 & \cdots & 0 & -x_1 \\ 1 & c_1 & -x_2 & \cdots & 0 & 0 \\ 1 & -x_1 & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & c_{q-2} & -x_2 \\ 1 & 0 & 0 & \cdots & -x_1 & c_{q-1} \end{vmatrix}}{\begin{vmatrix} c_0 & -x_2 & 0 & \cdots & 0 & -x_1 \\ -x_1 & c_1 & -x_2 & \cdots & 0 & 0 \\ 0 & -x_1 & c_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_{q-2} & -x_2 \\ -x_2 & 0 & 0 & \cdots & -x_1 & c_{q-1} \end{vmatrix}} \tag{D.1}$$

where $c_k = 1 - Q^k y_1 - Q^{-k} y_2$. In the following, we are interested in the case of $m_1 - m_2 = 0 \bmod q$ and $l_1 - l_2 = 0 \bmod q$, i.e. $m_1 - m_2$ and $l_1 - l_2$ are multiples of q.

$q = 2$

when $q = 2$, $Q = \exp\left(\frac{2i\pi}{2}\right) = -1$, we have

$$A_0 = A(x_1, x_2, y_1, y_2, -1) = \frac{1 + x_1 + x_2 + y_1 + y_2}{1 - (x_1 + x_2)^2 - (y_1 + y_2)^2}.$$

with $m_1 - m_2 = l_1 - l_2 = 0 \bmod 2$, A becomes

$$A_0 = A(x_1, x_2, y_1, y_2, -1) = \frac{1}{1 - (x_1 + x_2)^2 - (y_1 + y_2)^2}.$$

It is easy to read

$$\begin{aligned} Z_{m_1,m_2,l_1,l_2}(-1) &= \sum_{k_1=\min(m_1,m_2)}^{0,-2} \sum_{k_2=\min(l_1,l_2)}^{0,-2} \frac{m_1+m_2+l_1+l_2}{m_1+m_2+l_1+l_2} 2^{k_1+k_2} \\ &\quad \times \binom{\frac{m_1+m_2+l_1+l_2}{2}}{\frac{m_1-k_1}{2}, \frac{m_2-k_1}{2}, \frac{l_1-k_2}{2}, \frac{l_2-k_2}{2}, k_1, k_2} \\ &= \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-2} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-2} 2^{k_1+k_2} \binom{\frac{m_1+m_2+l_1+l_2}{2}}{\frac{m_1-k_1}{2}, \frac{m_2-k_1}{2}, \frac{l_1-k_2}{2}, \frac{l_2-k_2}{2}, k_1, k_2} \end{aligned} \tag{D.2}$$

And we already know that

$$Z_{m_1,m_2,l_1,l_2}(-1) = \binom{\lfloor (m_1+m_2+l_1+l_2)/2 \rfloor}{\lfloor (m_1+m_2)/2 \rfloor} \binom{m_1+m_2}{m_1} \binom{l_1+l_2}{l_1} \text{if } m_1{+}m_2 \text{ or } l_1{+}l_2 \text{ or both are even}$$

Hence, when $q=2$, $m_1-m_2=l_1-l_2=0 \bmod 2$, one find the identity:

$$\begin{aligned} \binom{\frac{m_1+m_2+l_1+l_2}{2}}{\frac{m_1+m_2}{2}} \binom{m_1+m_2}{m_1} \binom{l_1+l_2}{l_1} &= \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-2} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-2} 2^{k_1+k_2} \\ &\quad \binom{\frac{m_1+m_2+l_1+l_2}{2}}{\frac{m_1-k_1}{2}, \frac{m_2-k_1}{2}, \frac{l_1-k_2}{2}, \frac{l_2-k_2}{2}, k_1, k_2} \end{aligned}$$

dividing both sides by $(\frac{m_1+m_2+l_1+l_2}{2})!$, one finds:

$$\begin{aligned} \frac{\binom{m_1+m_2}{m_1}}{(\frac{m_1+m_2}{2})!} \frac{\binom{l_1+l_2}{l_1}}{(\frac{l_1+l_2}{2})!} &= \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-2} \frac{2^{k_1}}{(\frac{m_1-k_1}{2})!(\frac{m_2-k_1}{2})!k_1!} \\ &\quad \times \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-2} \frac{2^{k_2}}{(\frac{l_1-k_2}{2})!(\frac{l_2-k_2}{2})!k_2!} \end{aligned} \tag{D.3}$$

whith the change of variables: $m_1 = m_1 - a$, $m_2 = m_2 - a$,$l_1 = l_1 - b$, $l_2 = l_2 - b$, $k_1 = k_1 - a$ et $k_2 = k_2 - b$, one gets:

$$\begin{aligned} \frac{\binom{m_1+m_2-2a}{m_1-a}}{(\frac{m_1+m_2}{2}-a)!} \frac{\binom{l_1+l_2-2b}{l_1-b}}{(\frac{l_1+l_2}{2}-b)!} &= \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-2} \frac{2^{k_1}2^{-a}}{(\frac{m_1-k_1}{2})!(\frac{m_2-k_1}{2})!(k_1-a)!} \\ &\quad \times \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-2} \frac{2^{k_2}2^{-b}}{(\frac{l_1-k_2}{2})!(\frac{l_2-k_2}{2})!(k_2-b)!} \end{aligned} \tag{D.4}$$

$q = 3$

When $q=3$, $Q = \exp\left(\frac{2i\pi}{3}\right)$, we have

$$A_0 = A_3 = A\left(x_1, x_2, y_1, y_2, \exp\left(\frac{2i\pi}{3}\right)\right) = \frac{\begin{vmatrix} 1 & -x_2 & -x_1 \\ 1 & c_1 & -x_2 \\ 1 & -x_1 & c_2 \end{vmatrix}}{\begin{vmatrix} c_0 & -x_2 & -x_1 \\ -x_1 & c_1 & -x_2 \\ -x_2 & -x_1 & c_2 \end{vmatrix}}$$

$$= \frac{1 + x_1 + x_2 + y_1 + y_2 + x_1^2 + x_2^2 + y_1^2 + y_2^2 - x_1x_2 - y_1y_2 - Qx_1y_1 - Q^{-1}x_1y_2 - Q^{-1}x_2y_1 - Qx_2y_2}{1 - x_1^3 - x_2^3 - y_1^3 - y_2^3 - 3x_1x_2 - 3y_1y_2}$$

With the extra conditions $m_1 - m_2 = 0 \bmod 3$ and $l_1 - l_2 = 0 \bmod 3$, one can simplify A:

$$A\left(x_1, x_2, y_1, y_2, \exp\left(\frac{2i\pi}{3}\right)\right) = \frac{1 - x_1x_2 - y_1y_2}{1 - x_1^3 - x_2^3 - y_1^3 - y_2^3 - 3x_1x_2 - 3y_1y_2}$$

Developing A into a powe series and using the relation 2.9, one finds:

$$\begin{aligned}
Z_{m_1,m_2,l_1,l_2}\left(\exp\left(\frac{2i\pi}{3}\right)\right) = & \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-3} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-3} \binom{\frac{m_1+m_2+l_1+l_2+k_1+k_2}{3}}{\frac{m_1-k_1}{3}, \frac{m_2-k_1}{3}, \frac{l_1-k_2}{3}, \frac{l_2-k_2}{3}, k_1, k_2} 3^{k_1+k_2} \\
& - \sum_{\substack{k_1= \\ \min(m_1,m_2)-1}}^{0,-3} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-3} \binom{\frac{m_1+m_2+l_1+l_2+k_1+k_2-2}{3}}{\frac{m_1-k_1-1}{3}, \frac{m_2-k_1-1}{3}, \frac{l_1-k_2}{3}, \frac{l_2-k_2}{3}, k_1, k_2} 3^{k_1+k_2} \\
& - \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-3} \sum_{\substack{k_2= \\ \min(l_1,l_2)-1}}^{0,-3} \binom{\frac{m_1+m_2+l_1+l_2+k_1+k_2-2}{3}}{\frac{m_1-k_1}{3}, \frac{m_2-k_1}{3}, \frac{l_1-k_2-1}{3}, \frac{l_2-k_2-1}{3}, k_1, k_2} 3^{k_1+k_2}
\end{aligned}$$

with the change of variables: $k_1 + 1 = k_1$ for the second sum and $k_2 + 1 = k_2$ for the third sum above, one gets:

$$\begin{aligned}
Z_{m_1,m_2,l_1,l_2}\left(\exp\left(\frac{2i\pi}{3}\right)\right) = & \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-3} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-3} \binom{\frac{m_1+m_2+l_1+l_2+k_1+k_2}{3}}{\frac{m_1-k_1}{3}, \frac{m_2-k_1}{3}, \frac{l_1-k_2}{3}, \frac{l_2-k_2}{3}, k_1, k_2} 3^{k_1+k_2} \\
& - \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-3} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-3} \binom{\frac{m_1+m_2+l_1+l_2+k_1+k_2-1}{3}}{\frac{m_1-k_1}{3}, \frac{m_2-k_1}{3}, \frac{l_1-k_2}{3}, \frac{l_2-k_2}{3}, k_1 - 1, k_2} 3^{k_1+k_2-1} \\
& - \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-3} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-3} \binom{\frac{m_1+m_2+l_1+l_2+k_1+k_2-1}{3}}{\frac{m_1-k_1}{3}, \frac{m_2-k_1}{3}, \frac{l_1-k_2}{3}, \frac{l_2-k_2}{3}, k_1, k_2 - 1} 3^{k_1+k_2-1} \\
= & \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-3} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-3} \binom{\frac{m_1+m_2+l_1+l_2+k_1+k_2}{3}}{\frac{m_1-k_1}{3}, \frac{m_2-k_1}{3}, \frac{l_1-k_2}{3}, \frac{l_2-k_2}{3}, k_1, k_2} 3^{k_1+k_2} \\
& (1 - \frac{k_1}{m_1 + m_2 + l_1 + l_2 + k_1 + k_2} - \frac{k_2}{m_1 + m_2 + l_1 + l_2 + k_1 + k_2}) \\
= & \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-3} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-3} \frac{m_1 + m_2 + l_1 + l_2}{m_1 + m_2 + l_1 + l_2 + k_1 + k_2} 3^{k_1+k_2} \\
& \binom{\frac{m_1+m_2+l_1+l_2+k_1+k_2}{3}}{\frac{m_1-k_1}{3}, \frac{m_2-k_1}{3}, \frac{l_1-k_2}{3}, \frac{l_2-k_2}{3}, k_1, k_2}
\end{aligned}$$

$q = 4$

When $q = 4$, $Q = \exp\left(\frac{2i\pi}{4}\right) = \mathbf{i}$, we have:

$$A_0 = A_4 = A\left(x_1, x_2, y_1, y_2, \exp\left(\frac{2i\pi}{4}\right)\right) = \frac{\begin{vmatrix} 1 & -x_2 & 0 & -x_1 \\ 1 & c_1 & -x_2 & 0 \\ 1 & -x_1 & c_2 & -x_2 \\ 1 & 0 & -x_1 & c_3 \end{vmatrix}}{\begin{vmatrix} c_0 & -x_2 & 0 & -x_1 \\ -x_1 & c_1 & -x_2 & 0 \\ 0 & -x_1 & c_2 & -x_2 \\ -x_2 & 0 & -x_1 & c_3 \end{vmatrix}}$$

In the case: $m_1 - m_2 = 0 \bmod 4$ and $l_1 - l_2 = 0 \bmod 4$, simplify A:

$$A\left(x_1, x_2, y_1, y_2, \exp\left(\frac{2i\pi}{4}\right)\right) = \frac{1 - 2x_1x_2 - 2y_1y_2}{1 - {y_1}^4 - {y_2}^4 - {x_1}^4 - {x_2}^4 + 2{x_1}^2{x_2}^2 + 2{y_1}^2{y_2}^2 - 4y_1y_2 - 4x_1x_2}$$

Using the same method as before, one gets:

$$Z_{m_1,m_2,l_1,l_2}\left(\exp\left(\frac{2i\pi}{4}\right)\right) = \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-4} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-4} \sum_{k_3=k_1}^{0,-2} \sum_{k_4=k_2}^{0,-2} \frac{-2^{\frac{k_1+k_2-k_3-k_4}{2}} 4^{k_3+k_4}(m_1+m_2+l_1+l_2)}{m_1+m_2+l_1+l_2+2k_3+2k_4} \binom{\frac{m_1+m_2+l_1+l_2+2k_3+2k_4}{4}}{\frac{m_1-k_1}{4}, \frac{m_2-k_1}{4}, \frac{l_1-k_2}{4}, \frac{l_2-k_2}{4}, \frac{k_1-k_3}{2}, \frac{k_2-k_4}{2}, k_3, k_4}$$

In order to simplify this formula, one can use the results of the case $q = 2$ and identity D.4. First, rewriting $Z_{m_1,m_2,l_1,l_2}\left(\exp\left(\frac{2i\pi}{4}\right)\right)$:

$$\begin{aligned} Z_{m_1,m_2,l_1,l_2}\left(\exp\left(\frac{2i\pi}{4}\right)\right) &= \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-4} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-4} \sum_{\substack{k_3= \\ \min(m_1,m_2)}}^{0,-2} \sum_{\substack{k_4= \\ \min(l_1,l_2)}}^{0,-2} \frac{-2^{\frac{k_1+k_2-k_3-k_4}{2}}(m_1+m_2+l_1+l_2)}{m_1+m_2+l_1+l_2+2k_3+2k_4} \\ &\quad \binom{\frac{m_1+m_2+l_1+l_2+2k_3+2k_4}{4}}{\frac{m_1-k_1}{4}, \frac{m_2-k_1}{4}, \frac{l_1-k_2}{4}, \frac{l_2-k_2}{4}, \frac{k_1-k_3}{2}, \frac{k_2-k_4}{2}, k_3, k_4} \\ &= \sum_{\substack{k_3= \\ \min(m_1,m_2)}}^{0,-2} \sum_{\substack{k_4= \\ \min(l_1,l_2)}}^{0,-2} \frac{(-2)^{\frac{-(k_3+k_4)}{2}} 4^{k_3+k_4}(m_1+m_2+l_1+l_2)}{m_1+m_2+l_1+l_2+2k_3+2k_4} \frac{(\frac{m_1+m_2+l_1+l_2+2k_3+2k_4}{4})!}{k_3!k_4!} \\ &\quad \sum_{\substack{k_1= \\ \min(m_1,m_2)}}^{0,-4} \sum_{\substack{k_2= \\ \min(l_1,l_2)}}^{0,-4} \frac{(-2)^{\frac{k_1+k_2}{2}}}{\frac{(m_1-k_1)}{4}!\frac{(m_2-k_1)}{4}!\frac{(l_1-k_2)}{4}!\frac{(l_2-k_2)}{4}!\frac{(k_1-k_3)}{2}!\frac{(k_2-k_4)}{2}!} \\ &= \sum_{\substack{k_3= \\ \min(m_1,m_2)}}^{0,-2} \sum_{\substack{k_4= \\ \min(l_1,l_2)}}^{0,-2} \frac{(-2)^{\frac{-(k_3+k_4)}{2}} 4^{k_3+k_4}(m_1+m_2+l_1+l_2)}{m_1+m_2+l_1+l_2+2k_3+2k_4} \\ &\quad \times \frac{(\frac{m_1+m_2+l_1+l_2+2k_3+2k_4}{4})!}{k_3!k_4!} interm(m_1,m_2,l_1,l_2) \end{aligned} \tag{D.5}$$

where:

$$
\begin{aligned}
interm(m_1,m_2,l_1,l_2) &= \sum_{\substack{k_1=\\ \min(m_1,m_2)}}^{0,-4}\ \sum_{\substack{k_2=\\ \min(l_1,l_2)}}^{0,-4} \frac{(-2)^{\frac{k_1+k_2}{2}}}{\frac{(m_1-k_1)}{4}!\frac{(m_2-k_1)}{4}!\frac{(l_1-k_2)}{4}!\frac{(l_2-k_2)}{4}!\frac{(k_1-k_3)}{2}!\frac{(k_2-k_4)}{2}!} \\
&= \sum_{\substack{k_1=\\ \min(m_1,m_2)}}^{0,-4}\ \sum_{\substack{k_2=\\ \min(l_1,l_2)}}^{0,-4} \frac{(-1)^{\frac{\min(m_1,m_2)+\min(l_1,l_2)}{2}}2^{\frac{k_1+k_2}{2}}}{\frac{(m_1-k_1)}{4}!\frac{(m_2-k_1)}{4}!\frac{(l_1-k_2)}{4}!\frac{(l_2-k_2)}{4}!\frac{(k_1-k_3)}{2}!\frac{(k_2-k_4)}{2}!} \\
&= \sum_{\substack{k_1=\\ \min(m_1,m_2)}}^{0,-4} \frac{(-1)^{\frac{\min(m_1,m_2)}{2}}2^{\frac{k_1}{2}}}{\frac{(m_1-k_1)}{4}!\frac{(m_2-k_1)}{4}!\frac{k_1-k_3}{2}!} \sum_{\substack{k_1=\\ \min(m_1,m_2)}}^{0,-4} \frac{(-1)^{\frac{\min(l_1,l_2)}{2}}2^{\frac{k_2}{2}}}{\frac{(l_1-k_2)}{4}!\frac{(l_2-k_2)}{4}!\frac{k_2-k_4}{2}!}
\end{aligned}
$$

with the change of variables: $k_1/2 = k_1$ et $k_2/2 = k_2$:

$$
\begin{aligned}
&= \sum_{\substack{k_1=\\ \min(m_1,m_2)}}^{0,-2} \frac{(-1)^{\frac{\min(m_1,m_2)}{2}}2^{k_1}}{(\frac{m_1}{4}-\frac{k_1}{2})!(\frac{m_2}{4}-\frac{k_1}{2})!(k_1-\frac{k_3}{2})!} \\
&\times \sum_{\substack{k_1=\\ \min(m_1,m_2)}}^{0,-2} \frac{(-1)^{\frac{\min(l_1,l_2)}{2}}2^{k_2}}{(\frac{l_1}{4}-\frac{k_2}{2})!(\frac{l_2}{4}-\frac{k_2}{2})!(k_2-\frac{k_4}{2})!}
\end{aligned}
$$

with the identity D.4, one finds:

$$
interm(m_1,m_2,l_1,l_2) = \frac{2^{\frac{k_3+k_4}{2}}\binom{\frac{m_1+m_2}{2}-k_3}{\frac{m_1-k_3}{2}}\binom{\frac{l_1+l_2}{2}-k_4}{\frac{l_1-k_4}{2}}}{(\frac{m_1+m_2}{4}-\frac{k_3}{2})!(\frac{l_1+l_2}{4}-\frac{k_4}{2})!}(-1)^{\frac{\min(m_1,m_2)+\min(l_1,l_2)}{2}} \tag{D.6}
$$

Replacing $interm(m_1,m_2,l_1,l_2)$ by D.6, eq. (D.5) becomes:

$$
\begin{aligned}
Z_{m_1,m_2,l_1,l_2}\left(\exp\left(\frac{2i\pi}{4}\right)\right) = &\sum_{\substack{k_3=\\ \min(m_1,m_2)}}^{0,-2}\ \sum_{\substack{k_4=\\ \min(l_1,l_2)}}^{0,-2} \frac{(-2)^{\frac{-(k_3+k_4)}{2}}4^{k_3+k_4}(m_1+m_2+l_1+l_2)}{m_1+m_2+l_1+l_2+2k_3+2k_4} \\
&(-1)^{\frac{\min(m_1,m_2)+\min(l_1,l_2)}{2}}\frac{(\frac{m_1+m_2+l_1+l_2+2k_3+2k_4}{4})!}{k_3!k_4!} \\
&\frac{2^{\frac{k_3+k_4}{2}}}{(\frac{m_1+m_2}{4}-\frac{k_3}{2})!(\frac{l_1+l_2}{4}-\frac{k_4}{2})!}\binom{\frac{m_1+m_2-2k_3}{2}}{\frac{m_1-k_3}{2}}\binom{\frac{l_1+l_2-2k_4}{2}}{\frac{l_1-k_4}{2}} \\
= &\sum_{\substack{k_3=\\ \min(m_1,m_2)}}^{0,-2}\ \sum_{\substack{k_4=\\ \min(l_1,l_2)}}^{0,-2} \frac{4^{k_3+k_4}(m_1+m_2+l_1+l_2)}{m_1+m_2+l_1+l_2+2k_3+2k_4} \\
&(-1)^{\frac{\min(m_1,m_2)+\min(l_1,l_2)-k_3-k_4}{2}}\binom{\frac{m_1+m_2-2k_3}{2}}{\frac{m_1-k_3}{2}}\binom{\frac{l_1+l_2-2k_4}{2}}{\frac{l_1-k_4}{2}} \\
&\binom{\frac{m_1+m_2+l_1+l_2+2k_3+2k_4}{4}}{k_3,k_4,\frac{m_1+m_2}{4}-\frac{k_3}{2},\frac{l_1+l_2}{4}-\frac{k_4}{2}}
\end{aligned}
$$

Thus, $Z_{m_1,m_2,l_1,l_2}\left(\exp\left(\frac{2i\pi}{4}\right)\right)$ can be simplified as:

$$Z_{m_1,m_2,l_1,l_2}\left(\exp\left(\frac{2i\pi}{4}\right)\right) = \sum_{\substack{k_3= \\ \min(m_1,m_2)}}^{0,-2} \sum_{\substack{k_4= \\ \min(l_1,l_2)}}^{0,-2} \frac{4^{k_3+k_4}(m_1+m_2+l_1+l_2)}{m_1+m_2+l_1+l_2+2k_3+2k_4}$$
$$(-1)^{\frac{\min(m_1,m_2)+\min(l_1,l_2)-k_3-k_4}{2}} \binom{\frac{m_1+m_2-2k_3}{2}}{\frac{m_1-k_3}{2}} \binom{\frac{l_1+l_2-2k_4}{2}}{\frac{l_1-k_4}{2}}$$
$$\binom{\frac{m_1+m_2+l_1+l_2+2k_3+2k_4}{4}}{k_3, k_4, \frac{m_1+m_2}{4}-\frac{k_3}{2}, \frac{l_1+l_2}{4}-\frac{k_4}{2}}$$

Appendix

E Deriving eq. (3.31) from eq. (3.28)

From eq. (3.28), the generating function of $\mathrm{Tr}\left(H^{(\lambda)}_{2\pi p/q}\right)^n$ can be written as

$$\sum_{n\geq 0}\mathrm{Tr}\left(H^{(\lambda)}_{2\pi p/q}\right)^n z^n = \frac{1}{q}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\sum_r \frac{E}{E-E_r(k_x,k_y)} \tag{E.1}$$

with $E = 1/z$. The eigenvalues $E^{(\lambda)}_r(k_x,k_y)$ are q roots of

$$f(E) = E^q b^{(\lambda)}_{p/q}(1/E) = 2(\cos qk_x + \Lambda\cos qk_y)$$

where $\Lambda = (\lambda/2)^q$, then

$$f(E) - 2(\cos qk_x + \Lambda\cos qk_y) = \prod_r (E - E^{(\lambda)}_r(k_x,k_y)).$$

Therefore

$$\frac{f'(E)}{f(E)-2(\cos qk_x+\Lambda\cos qk_y)} = \sum_r \frac{1}{E-E^{(\lambda)}_r(k_x,k_y)}$$

Putting this equation into $(E.1)$, we get

$$\sum_{n\geq 0}\mathrm{Tr}\left(H^{(\lambda)}_{p/q}\right)^n z^n = \frac{E}{q}\frac{f'(E)}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dk_x dk_y \frac{1}{f(E)-2(\cos qk_x+\Lambda\cos qk_y)} \tag{E.2}$$

Evaluating the first integral of k_x

$$\int_{-\pi}^{\pi}\frac{dk_x}{f(E)-2(\cos qk_x+\Lambda\cos qk_y)} \overset{u=qk_x}{=} \frac{1}{q}\int_{-q\pi}^{q\pi}\frac{du}{f(E)-2(\cos u+\Lambda\cos qk_y)}$$

the period of $\frac{1}{f(E)-2(\cos u+\Lambda\cos qk_y)}$ is 2π, equation above becomes $\int_{-q\pi}^{-q\pi+2\pi}\frac{du}{f(E)-2(\cos u+\Lambda\cos qk_y)}$. Translate the domaine of integration so that $\tan\left(\frac{u}{2}\right)$ is continuous on this interval :

$$\begin{aligned}\int_{-\pi}^{\pi}\frac{du}{f(E)-2(\cos u+\Lambda\cos qk_y)} &\overset{x=\tan\left(\frac{u}{2}\right)}{=} \int_{-\infty}^{\infty}\frac{2dx}{(1+x^2)(f(E)-2\frac{(1-x^2)}{x^2+1}-2\Lambda\cos qk_y)}\\ &= \int_{-\infty}^{\infty}\frac{2dx}{(f(E)-2\Lambda\cos qk_y-2)\left(1+\frac{f(E)-2\Lambda\cos qk_y+2}{f(E)-2\Lambda\cos qk_y-2}x^2\right)}\\ &= \frac{2}{f(E)-2\Lambda\cos qk_y-2}\int_{-\infty}^{\infty}\frac{dx}{1+\frac{f(E)-2\Lambda\cos qk_y+2}{f(E)-2\Lambda\cos qk_y-2}x^2}\end{aligned}$$

with $p = \sqrt{\frac{f(E)-2\Lambda\cos qk_y+2}{f(E)-2\Lambda\cos qk_y-2}}x$

$$
\begin{aligned}
&= \frac{2}{\sqrt{(f(E)-2\Lambda\cos qk_y)^2-4}}\int_{-\infty}^{\infty}\frac{dp}{1+p^2}\\
&= \frac{2}{\sqrt{(f(E)-2\Lambda\cos qk_y)^2-4}}2\lim_{a\to\infty}\tan^{-1}(p)|_{p=0}^{p=a}\\
&= \frac{2\pi}{\sqrt{(f(E)-2\Lambda\cos qk_y)^2-4}}
\end{aligned}
$$

puting this into $(E.2)$, one gets

$$
\begin{aligned}
&\sum_{n\geq 0}\mathrm{Tr}\left(H^{(\lambda)}_{p/q}\right)^n z^n = \frac{E}{q}\frac{f'(E)}{2\pi}\int_{-\pi}^{\pi}\frac{dk_y}{\sqrt{(f(E)-2\Lambda\cos qk_y)^2-4}}\\
&\overset{t=qk_y}{=} \frac{E}{q^2}\frac{f'(E)}{2\pi}\int_{-q\pi}^{q\pi}\frac{dt}{\sqrt{(f(E)-2\Lambda\cos t)^2-4}}\\
&= \frac{E}{q}\frac{f'(E)}{2\pi}\int_{-q\pi}^{-q\pi+2\pi}\frac{dt}{\sqrt{(f(E)-2\Lambda\cos t)^2-4}}\\
&= \frac{E}{q}\frac{f'(E)}{2\pi}\int_{-\pi}^{\pi}\frac{dt}{\sqrt{(f(E)-2\Lambda\cos t)^2-4}}\\
&= \frac{E}{q}\frac{f'(E)}{\pi}\int_{0}^{\pi}\frac{dt}{\sqrt{(f(E)-2\Lambda\cos t-2)(f(E)-2\Lambda\cos t+2)}}\\
&= \frac{E}{q}\frac{f'(E)}{\pi}\int_{0}^{\pi}\frac{(1+\tan^2(\frac{t}{2}))dt}{\sqrt{(f(E)-2\Lambda-2+(f(E)+2\Lambda-2)\tan^2(\frac{t}{2}))(f(E)-2\Lambda+2+(f(E)+2\Lambda+2)\tan^2(\frac{t}{2}))}}
\end{aligned}
$$

change of variable : $\sqrt{\frac{f[E]-2\Lambda-2}{f[E]+2\Lambda-2}}\tan y = \tan\left(\frac{t}{2}\right)$

$$
\begin{aligned}
&= \frac{E}{q}\frac{f'(E)}{\pi}\int_{0}^{\frac{\pi}{2}}\frac{2(1+\tan^2 y)\quad dy}{\sqrt{(1+\tan^2 y)(f(E)^2-(2\Lambda-2)^2+(f(E)+2\Lambda+2)(f[E]-2\Lambda-2)\tan^2 y)}}\\
&= \frac{2E}{q}\frac{f'(E)}{\pi}\int_{0}^{\frac{\pi}{2}}\frac{\sqrt{1+\tan^2 y}\quad dy}{\sqrt{f(E)^2-(2\Lambda-2)^2+(f(E)^2-(2\Lambda+2)^2)\tan^2 y}}\\
&= \frac{2E}{q}\frac{f'(E)}{\pi}\int_{0}^{\frac{\pi}{2}}\frac{dy}{\sqrt{f(E)^2-(2\Lambda-2)^2-16\Lambda\sin^2 y}}\\
&= \frac{2E}{q\pi}\frac{f'(E)}{\sqrt{f(E)^2-(2\Lambda-2)^2}}\int_{0}^{\frac{\pi}{2}}\frac{dy}{\sqrt{1-\frac{16\Lambda}{f(E)^2-(2\Lambda-2)^2}\sin^2(y)}}\\
&= \frac{2E}{q\pi}\frac{f'(E)}{\sqrt{f(E)^2-(2\Lambda-2)^2}}K\left(\frac{16\Lambda}{f(E)^2-(2\Lambda-2)^2}\right)
\end{aligned}
$$

where $K(x)=\int_0^{\frac{\pi}{2}}\frac{d\theta}{\sqrt{1-x\sin^2\theta}}$ is the elliptic Integral of the first kind. Thus, we get

$$
\sum_{n\geq 0}\mathrm{Tr}\left(H^{(\lambda)}_{2\pi p/q}\right)^n z^n = \frac{2E}{q\pi}\frac{f'(E)}{\sqrt{f(E)^2-(2\Lambda-2)^2}}K\left(\frac{16\Lambda}{f(E)^2-(2\Lambda-2)^2}\right)
$$

which is equivalent to eq. (3.31).