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On the spectrum of a random walk on the discrete Heisenberg group and the norm of Harper's operator

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Abstract

Harper's operator is the self-adjoint operator on $l^2(\mathbb{Z})$ defined by $H_{\theta,\phi}\xi(n) = \xi(n+1) + \xi(n-1) + 2\cos(2\pi(n\theta+\phi))\xi(n)$ ($\xi \in l^2(\mathbb{Z})$, $n \in \mathbb{Z}$, $\theta, \phi \in [0, 1]$). We first show that the determination of the spectrum of the transition operator on the Cayley graph of the discrete Heisenberg group in its standard presentation, is equivalent to the following upper bound on the norm of $H_{\theta,\phi}$: $\|H_{\theta,\phi}\| \leq 2(1 + \sqrt{2} + \cos(2\pi\theta))$. We then prove this bound by reducing it to a problem on periodic Jacobi matrices, viewing $H_{\theta,\phi}$ as the image of $H_\theta = U_\theta + U_\theta^* + V_\theta + V_\theta^*$ in a suitable representation of the rotation algebra $\mathcal{A}_\theta$. We also use powers of H_θ to obtain various upper and lower bounds on $\|H_\theta\| = \max_\phi \|H_{\theta,\phi}\|$. We show that "Fourier coefficients" of $H_\theta{}^k$ in $\mathcal{A}_\theta$ have a combinatorial interpretation in terms of paths in the square lattice $\mathbb{Z}^2$. This allows us to give some applications to asymptotics of lattice paths combinatorics.

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0. Introduction

For a finitely generated group Γ endowed with a finite generating subset S which is symmetric ($S = S^{-1}$), we consider the Markov or transition operator h_S on $l^2(\Gamma)$ given

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by $h_S\xi(x) = (1/|S|)\sum_{s\in S}\xi(xs)$ (this is the transition operator associated with the simple nearest neighbour random walk on the Cayley graph $\mathcal{G}(\Gamma, S)$, [1] i.e. the random walk starting from the origin and, at each step, moving with equal probability from one vertex to one of its neighbours). It is known since the work of Kesten [Kes59b,Kes59a] that the spectrum of the self-adjoint operator h_S contains much information about the pair (Γ, S). For example, one has $\|h_S\| = 1$ iff Γ is amenable; if one can write $S = S^+ \amalg (S^+)^{-1}$ (disjoint union), with $|S^+| = n$, then $\sqrt{2n-1}/n \leq \|h_S\|$ and, provided $n \geq 2$, equality holds iff Γ is the free group on S^+; in that case one has

$$Sp\, h_S = \left[-\frac{\sqrt{2n-1}}{n}, \frac{\sqrt{2n-1}}{n}\right].$$

See [HRV93a,HRV93b] for other results relating spectral properties of h_S to group theoretical properties of (Γ, S). However, for infinite groups there are relatively few cases where exact computations of spectra of transition operators have been performed (not to mention the computation of the spectral mesure, that would be the next step). We are basically aware of two classes of groups where this was done: virtually abelian groups, where one reduces to an abelian group of finite index and then uses Fourier analysis techniques, and virtually free groups, where one can appeal to the combinatorics of trees. The paper [CV] illustrates the difficulty of treating other non-amenable examples like surface groups.

In this paper we consider a classical example of a step 2 nilpotent group: the discrete Heisenberg group

$$H(\mathbb{Z}) = \left\{ \begin{pmatrix} 1 & m & p \\ 0 & 1 & n \\ 0 & 0 & 1 \end{pmatrix} \mid m, n, p \in \mathbb{Z} \right\}$$

with generating subset

$$S = \left\{ x^{\pm 1} = \begin{pmatrix} 1 & \pm 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, y^{\pm 1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \pm 1 \\ 0 & 0 & 1 \end{pmatrix}, z^{\pm 1} = \begin{pmatrix} 1 & 0 & \pm 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}.$$

For the corresponding operator h_S, we prove:

Proposition 3. *$Sp\, h_S$ is an interval $[m, 1]$ with $m = \frac{1}{3}(-1-\sqrt{2}) = -0.804737854\ldots$*

The value of m was obtained by relating h_S to Harper's operator.

Harper's operator is the operator $H_{\theta,\phi}$ $(\theta, \phi \in [0, 1])$ on $l^2(\mathbb{Z})$ given by $(H_{\theta,\phi}\xi)(n) = \xi(n+1) + \xi(n-1) + 2\cos 2\pi(n\theta + \phi)\cdot\xi(n)$ $(\xi \in l^2(\mathbb{Z}), n \in \mathbb{Z})$. It is one of the most studied discrete Schrödinger operator, both in the physics and mathematics literature (see [Bel91,Shu94] for recent surveys). An impressive wealth of numerical data is available

[1] Recall that $\mathcal{G}(\Gamma, S)$ is the graph with set Γ of vertices, and set $\{\{x, xs\}: x \in \Gamma, s \in S\}$ of edges.

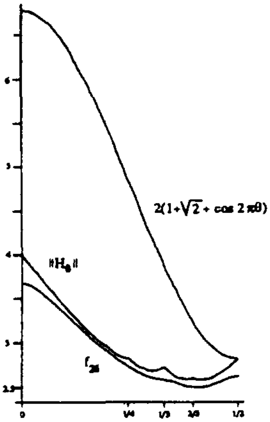


Fig. 1. The functions $\theta \longmapsto f_{26}(\theta)$, $\theta \longmapsto \|H_\theta\|$, $\theta \longmapsto 2(1+2^{1/2}+\cos 2\pi\theta)$.

concerning the spectrum of $H_{\theta,\phi}$ (leading in particular to the famous "Hofstadter butterfly" [Hof 76]). We will first show that our Proposition 3 is equivalent to:

Proposition 4. *For any* $\theta, \phi \in [0,1]$, $\|H_{\theta,\phi}\| \leq 2(1+\sqrt{2}+\cos(2\pi\theta))$ *with equality for* $\theta = \frac{1}{2}$, $\phi = 0$.

For θ irrational, $\|H_{\theta,\phi}\|$ does not depend on ϕ (see [Rie81]), but it does for θ rational. One may unify both cases by considering the two-dimensional Schrödinger operator H_θ on $l^2(\mathbb{Z}^2)$ defined by

$$H_\theta\xi(m,n) = \xi(m+1,n) + \xi(m-1,n) + \mathrm{e}^{\mathrm{i}\theta m}\xi(m,n-1) + \mathrm{e}^{-\mathrm{i}\theta m}\xi(m,n+1)$$
$$\xi \in l^2(\mathbb{Z}^2),\ m,n \in \mathbb{Z}.$$

For any θ, one has (see [Bel91], or Lemma 3 below) $\|H_\theta\| = \max_\phi \|H_{\theta,\phi}\|$ so that the Proposition 4 is equivalent to $\|H_\theta\| \leq 2(1+\sqrt{2}+\cos(2\pi\theta))$, with equality at $\theta = \frac{1}{2}$.

Figure 1 gives striking experimental evidence for that statement; but one has to be aware that the curve $\theta \longmapsto \|H_\theta\|$ was plotted by computing $\|H_\theta\|$ for some rational values of θ, and then linearly interpolating, so that there is really something to prove in Proposition 4. The fact that the function $\theta \longmapsto \|H_\theta\|$ is quite irregular (however continuous) causes difficulties in tackling Proposition 4 with the classical tools of calculus, so that our approach will be mainly C^*-algebraic. We first view h_S as an element of the reduced C^*-algebra [2] $C^*_r(\Gamma)$. Now, since $\Gamma = H(\mathbb{Z})$ is amenable, $C^*_r(\Gamma)$ is $*$-isomorphic to the full C^*-algebra $C^*(\Gamma)$, which is the universal C^*-algebra generated by three unitaries x, y, z satisfying the commutation rule $x \cdot y = z \cdot y \cdot x$ with z central. For each $\theta \in [0,1]$, denote by $\mathcal{A}_\theta$ Rieffel's rational or irrational rotation algebra [Rie81,Rie90], i.e. the universal C^*-algebra generated by two unitaries U_θ,

[2] That is the C^*-algebra generated by the left regular representation of Γ on $l^2(\Gamma)$.

V_θ satisfying the commutation rule $V_\theta U_\theta = e^{2\pi i\theta} U_\theta V_\theta$. We may view the operator H_θ as the element $U_\theta + U_\theta^* + V_\theta + V_\theta^*$ in $\mathcal{A}_\theta$ (this is a key fact in the C^*-algebraic approach to H_θ, see e.g. [RB90,CEY90]). There is an obvious $*$-homomorphism π_θ from $C^*(\Gamma)$ onto $\mathcal{A}_\theta$, defined by $\pi_\theta(x) = U_\theta$, $\pi_\theta(y) = V_\theta$, $\pi_\theta(z) = e^{-2\pi i\theta} \cdot \mathbf{1}$. Moreover, $\pi_\theta(h_S) = \frac{1}{6}(H_\theta + 2\cos 2\pi\theta)$; the fact that $(\pi_\theta)_{\theta\in[0,1]}$ is a separating family of representation then explains the link between the spectrum of h_S and the spectrum of the H_θ's.

Our paper is organized as follows. In Section 1 we digress on the Kaplansky–Kadison conjecture of idempotents for reduced C^*-algebras of torsion-free discrete groups, and explain its relevance to simplify computations of spectra of transition operators (it asserts that such spectra are intervals); we also give a new proof of this conjecture for torsion-free finitely generated nilpotent groups (in particular for $H(\mathbb{Z})$).

In Section 2, we elaborate on the above connection between the operator $h_S \in C^*(H(\mathbb{Z}))$ and Harper's operator, and we establish the equivalence between Propositions 3 and 4.

In Section 3 we prove Proposition 4.

In Section 4, we look at powers of H_θ in $\mathcal{A}_\theta$; this enables us to give other upper bounds on the function $\theta \longrightarrow \|H_\theta\|$. Powers of H_θ are linear combinations of monomials $U_\theta^m V_\theta^n$, whose coefficients have a combinatorial meaning in terms of paths from the origin in the square lattice $\mathbb{Z}^2$. In particular, for $m = n = 0$, one gets the canonical trace of H_θ^{2k} as a trigonometric polynomial $f_k^{2k}(\theta)$ whose lth coefficient is the number of closed paths through $(0, 0)$ in $\mathbb{Z}^2$, with length $2k$ and enclosed oriented area l. We also show that the family of C^∞-functions $f_k(\theta)$ approximates uniformly and from below the irregular function $\theta \longmapsto \|H_\theta\|$. The function f_{26} is also plotted in Fig. 1.

In Section 5, we give combinatorial applications of the results of Section 4, first to a family of 6-regular finite graphs covered by $\mathcal{G}(\Gamma, S)$, second to lattice paths combinatorics in $\mathbb{Z}^2$: we give asymptotic behaviours for the logarithms of a number of expressions involving the number of closed paths of length $2k$ with area satisfying congruence relations modulo a fixed argument. For example, if $N(2k)^{\mathrm{ev}}$ (resp. $N(2k)^{\mathrm{odd}}$) denotes the number of closed paths through $(0, 0)$ with length $2k$ and even (resp. odd) enclosed area, we have that $\log(N(2k)^{\mathrm{ev}} - N(2k)^{\mathrm{odd}})$, behaves asymptotically like $k \log 8$.

1. A digression on the conjecture of idempotents

The conjecture of idempotents or Kaplansky–Kadison conjecture states that the reduced C^*-algebra $C_r^*(\Gamma)$ of a torsion free group Γ has no non-trivial idempotent (see [Val89] for a survey). For Γ a finitely generated, torsion free nilpotent group we know of at least four different proofs of this conjecture : via K-theory [Ros83], via harmonic analysis [KT89], via C^*-algebra theory [JP90] and via cyclic cohomology [Ji92]. In the special case of $H(\mathbb{Z})$, there is a proof due to Bellissard [Bel88] with a non-commutative differential flavour (Streda's formula). We propose one more proof so that the result has a chance of being correct.

Proposition 1. *Let Γ be a finitely generated torsion-free nilpotent group. Then $C_r^*(\Gamma)$ has no idempotent except* 0 *and* 1.

Proof. Let G be a connected Lie group; Kasparov has defined the commutative ring $R(G)$ of Fredholm representations of G (see [Kas88]). $R(G)$ is a unital ring, with a distinguished idempotent γ_G such that $\gamma_G R_G$ is isomorphic, via restriction, to the representation ring $R(K)$ of the maximal compact subgroup K of G. The element $1 - \gamma_G$ of $R(G)$ is the celebrated Kasparov obstruction of G. It is known [BC82,Val89] that if $1 - \gamma_G = 0$, then the Kaplansky–Kadison conjecture holds for any torsion-free discrete subgroup of G. On the other hand, it is a fundamental result of Kasparov that $1 - \gamma_G = 0$ if G is amenable (e.g. nilpotent). Now, let Γ be a finitely generated, torsion-free nilpotent group, and let G be the Malcev completion of Γ, i.e. the unique connected nilpotent Lie group in which Γ embeds as a lattice [3] (see [Rag79]). It follows from the previous remark that $1 - \gamma_G = 0$, so that the Kaplansky–Kadison conjecture holds for Γ. □

The link between the conjecture of idempotents and spectral properties of elements in $C_r^*(\Gamma)$is provided by the following easy lemma.

Lemma 1. *Let A be a unital Banach algebra, the following properties are equivalent:*
(i) *A has no idempotent except* 0 *and* 1.
(ii) *The spectrum of every element in A is connected.*
If moreover A is a C^*-algebra, this is still equivalent to:
(iii) *The spectrum of every self-adjoint element of A is an interval.*

Proof. For (i)⇔(ii) use holomorphic functional calculus; if A is a C^*-algebra then (ii)⇒(iii) is clear, and (iii)⇒(i) follows from the fact that any idempotent in A is equivalent to a self-adjoint idempotent. □

2. From the spectrum of a random walk on $H(\mathbb{Z})$ to the norm of Harper's operator

From now on, we denote by Γ the Heisenberg group $H(\mathbb{Z})$. The group Γ admits two natural presentations :

$$\begin{aligned}\Gamma &= \langle x, y\colon [x,[x,y]] = [y,[y,x]] = 1\rangle \\ &= \langle x, y, z\colon z = [x,y], [x,z] = [y,z] = 1\rangle .\end{aligned}$$

It is a simple exercise to compute the spectrum of the Markov operator associated with the first presentation, i.e. the transition operator on the Cayley graph $\mathcal{G}(\Gamma, S_0)$ with $S_0 = \{x, y, x^{-1}, y^{-1}\}$. This operator is $h_{S_0} = \frac{1}{4}(x + y + x^{-1} + y^{-1}) \in C_r^*(\Gamma)$.

Lemma 2. $Sp(h_{S_0}) = [-1, 1]$.

Proof. Let $Z(\Gamma)$ be the centre of Γ; the quotient map $\alpha\colon \Gamma \longrightarrow \Gamma/Z(\Gamma) \simeq \mathbb{Z}^2$ does induce a $*$-homomorphism $\widetilde{\alpha}$ from $C_r^*(\Gamma)$ onto $C^*(\mathbb{Z}^2)$. Then $\widetilde{\alpha}(h_{S_0}) = \frac{1}{4}(\alpha(x)+\alpha(x^{-1})+\alpha(y)+\alpha(y^{-1}))$; since $\{\alpha(x), \alpha(y)\}$ is the canonical basis of $\mathbb{Z}^2$, it is an elementary exercise on

[3] For $\Gamma = H(\mathbb{Z})$, G is the standard three-dimensional Heisenberg group.

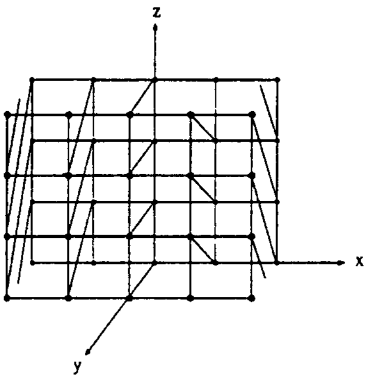


Fig. 2.

Fourier transform that $Sp(\widetilde{\alpha}(h_{S_0})) = [-1, 1]$. Then $[-1, 1] \subseteq Sp(h_{S_0})$ and since $\|h_{S_0}\| \leq 1$, equality holds. □

We now consider the spectrum of the Markov operator associated with the second presentation of Γ (this presentation is well suited to the embedding of Γ as a lattice in the three-dimensional real Heisenberg group). Set $S = \{x, y, z, x^{-1}, y^{-1}, z^{-1}\}$; the Cayley graph $\mathcal{G}(\Gamma, S)$ is sketched in Fig. 2.

The transition operator is $h_S = \frac{1}{6}(x + y + z + x^{-1} + y^{-1} + z^{-1}) \in C_r^*(\Gamma)$. One of our motivating questions was: how does the spectrum change when h_{S_0} is replaced by h_S, i.e. when the extra generator z is added.

Proposition 2. *$Sp(h_S)$ is an interval $[m, 1]$ with $-1 < m$.*

Proof. By Proposition 1, there is no non-trivial idempotent in $C_r^*(\Gamma)$ so that, by Lemma 1, $Sp(h_S)$ is an interval $[m, M]$ with $-1 \leq m \leq M \leq 1$ (because $\|h_S\| \leq 1$). Since Γ is amenable, one has $1 \in Sp(h_S)$ by Kesten's characterization of amenability [Kes59b,Kes59a]. Finally, one has $-1 < m$ because the graph $\mathcal{G}(\Gamma, S)$ is not bipartite (see [HRV93a, Proposition 5.2]). □

We will ultimately get the following value for m.

Proposition 3. $m = \frac{1}{3}(-1 - \sqrt{2}) = -0.804737854\ldots$

Recall from the introduction that, for any $\theta \in [0, 1]$, the C^*-algebra $\mathcal{A}_\theta$ appears as a quotient of $C^*(\Gamma)$ via the map

$$\pi_\theta : \begin{cases} C^*(\Gamma) & \longrightarrow & \mathcal{A}_\theta \\ x & \longmapsto & U_\theta \\ y & \longmapsto & V_\theta \\ z & \longmapsto & \mathrm{e}^{-2\pi \mathrm{i}\theta} \end{cases}$$

The family of representations $(\pi_\theta)_{\theta\in[0,1]}$ of $C^*(\Gamma)$ is separating, so that for any self-adjoint element h of $C^*(\Gamma)$, one has

$$Sp(h) = \overline{\bigcup_{\theta\in[0,1]} Sp(\pi_\theta(h))} \tag{1}$$

(the relevance of the $\mathcal{A}_\theta$'s in the representation theory of $C^*(\Gamma)$ was one of Rieffel's motivation in [Rie81]). For $\theta \in [0, 1]$, one has

$$\pi_\theta(h_S) = \tfrac{1}{6}\left[U_\theta + U_\theta^* + V_\theta + V_\theta^* + 2\cos 2\pi\theta\right].$$

In the faithful representation of $\mathcal{A}_\theta$ on $l^2(\mathbb{Z}^2)$ given by $U_\theta\xi(m,n) = \xi(m-1,n)$ and $V_\theta\xi(m,n) = \mathrm{e}^{2\pi \mathrm{i}\theta m}\xi(m,n-1)$, the self-adjoint operator $U_\theta + U_\theta^* + V_\theta + V_\theta^*$ is mapped precisely to the operator H_θ from the introduction, so from now on we set $H_\theta = U_\theta + U_\theta^* + V_\theta + V_\theta^*$. Plotting $Sp(H_\theta)$ against θ reveals numerically an amazing butterfly-like structure, first observed by Hofstadter [Hof 76]. Among the qualitative results proved about $Sp(H_\theta)$, we quote the following :

- For $\theta = p/q$ (p, q coprime integers), $Sp(H_\theta)$ is a band spectrum consisting of either $q-1$ intervals (for q even) or q intervals (for q odd): see [CEY90], and Remark (3) in Section 3.
- For a set of irrational θ's with Lebesgue measure 1, $Sp(H_\theta)$ is a Cantor set with measure 0; see [Las94] (note that it is a famous conjecture of Marc Kac, known as the Ten Martinis problem, that this holds for any [4] irrational θ).

According to formula (1), to compute $Sp(h_S)$ we have in principle to consider $Sp(H_\theta)$, shift it by $2\cos 2\pi\theta$, take the union of these sets over all θ's, and form the closure. But actually, this is asking for too much, since by Proposition 2 we a priori know that $Sp(h_S)$ is an interval. If $m(\theta)$ denotes the bottom of the spectrum of H_θ, we have $m = \inf_{\theta\in[0,1]} \frac{1}{6}(m(\theta) + 2\cos(2\pi\theta))$. By symmetry of $Sp(H_\theta)$ [5] we have $m(\theta) = -\|H_\theta\|$ and therefore

$$-m = \sup_{\theta\in[0,\frac{1}{2}]} \tfrac{1}{6}(\|H_\theta\| - 2\cos(2\pi\theta)) \tag{2}$$

(the restriction to $[0, \frac{1}{2}]$ is due to the $*$-automorphism

$\mathcal{A}_\theta \to \mathcal{A}_{1-\theta}$: $\begin{cases} U \mapsto V \\ V \mapsto U \end{cases}$ that maps H_θ to $H_{1-\theta}$).

The following facts are known about the function $\theta \longmapsto \|H_\theta\|$ (which describes the boundary of Hofstadter's butterfly):

- It is continuous [Ell82]; in particular the supremum in (2) is attained.
- It is Lipschitz continuous [Bel94] [6], in particular $\theta \longmapsto H_\theta$ is almost everywhere differentiable.

[4] Last probably deserves 9.9999... of the ten Martinis...

[5] The involutive $*$-automorphism of $\mathcal{A}_\theta$ given by $\begin{cases} U \longmapsto -U \\ V \longmapsto -V \end{cases}$ maps H_θ to $-H_\theta$.

[6] Bellissard conjectures that $\theta \longmapsto H_\theta$ is differentiable at any irrational θ. Note that there is no known estimate on the Lipschitz constant; by way of contrast, Avron et al., [AMS90, Proposition 7.1] earlier

– It is not differentiable at any rational values of θ although it admits there a left and a right derivative; this follows from the "Wilkinson–Rammal formula" (see [RB90,HS90]).

The lack of regularity of the function $\theta \longmapsto H_\theta$ makes the computation of the maximum of $\theta \longmapsto \|H_\theta\| - 2\cos 2\pi\theta$ quite difficult. We first solved this extremal problem graphically, getting the empirical result that the maximum is attained at $\theta = \frac{1}{2}$. Now it is an easy exercise on 2×2-matrices to compute $Sp(H_{1/2})$ and to get $\|H_{1/2}\| = 2\sqrt{2}$. So the experimental result, that will be eventually proved in the next section, is:

Proposition 4. $\max_{\theta\in[0,1/2]}(\|H_\theta\| - 2\cos 2\pi\theta) \le 2(1+\sqrt{2})$ *with equality at* $\theta = \frac{1}{2}$.

In other words: for any $\theta \in [0, \frac{1}{2}]$, $\|H_\theta\| \le 2(1+\sqrt{2}+\cos 2\pi\theta)$. In view of (2), Propositions 3 and 4 are equivalent.

3. Validity of the upper bound on $\|H_\theta\|$

First, let us recall that for $\theta = p/q \in [0,1]$ rational, there is a faithful representation of $\mathcal{A}_{p/q}$ as a matrix algebra over the torus: $\mathcal{A}_{p/q}$ is the C^*-subalgebra of $\mathcal{M}_q(C(\mathbb{T}))$ (the $q \times q$ matrices with coefficients in the continous functions on the two-dimensional torus) generated by:

$$M_U(z_1,z_2) = z_1 \cdot \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & \rho & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \rho^{q-1} \end{pmatrix}, \quad M_V(z_1,z_2) = z_2 \cdot \begin{pmatrix} 0 & \dots & 0 & 1 \\ 1 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 1 & 0 \end{pmatrix}$$

with $\rho = \mathrm{e}^{2\pi i\theta}$ and $(z_1,z_2) \in \mathbb{T}^2$. The operator $H_{p/q}$ is then identified with the family of periodic Jacobi matrices:

$$M_H(z_1,z_2) = \begin{pmatrix} z_1+\overline{z_1} & \overline{z_2} & 0 & \cdots & 0 & z_2 \\ z_2 & \rho z_1+\overline{\rho z_1} & \overline{z_2} & \cdots & 0 & 0 \\ 0 & z_2 & \rho^2 z_1+\overline{\rho^2 z_1} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \rho^{q-2}z_1+\overline{\rho^{q-2}z_1} & \overline{z_2} \\ \overline{z_2} & 0 & 0 & \cdots & z_2 & \rho^{q-1}z_1+\overline{\rho^{q-1}z_1} \end{pmatrix}.$$

At this point, we explain the link with Harper's operator $H_{\theta,\phi}$ mentioned in the introduction. For $\theta = p/q$, the operator $H_{\theta,\phi}$ is periodic of period q, meaning that it takes the form

obtained the weaker statement that $\theta \longmapsto H_\theta$ is Hölder continous of exponent $\frac{1}{2}$, with the explicit constant $6\sqrt{2}$.

of a $q \times q$ scalar matrix in the decomposition $l^2(\mathbb{Z}) = \bigoplus_{i=0}^{q-1} l^2(q\mathbb{Z} + i)$. Now this matrix is precisely $M_H(\mathrm{e}^{2\pi \mathrm{i}\phi}, 1)$. We want to prove:

Proposition 4. $\max_{\theta \in [0,1/2]}(\|H_\theta\| - 2\cos 2\pi\theta) \le 2(1+\sqrt{2})$.

Using the continuity of the function $\theta \longmapsto \|H_\theta\|$ it will be enough to show that $\|H_\theta\| - 2\cos 2\pi\theta \le 2(1+\sqrt{2})$ for any rational θ. We will need the following lemma.

Lemma 3. *For $\theta = p/q$, the maximum of $\|M_H(z_1, z_2)\|$ is attained for $z_1 = z_2 = 1$. In other words, one has $\|H_\theta\| = \|H_{\theta,0}\|$.*

Proof. The norm of $M_H(z_1, z_2)$ is given by the maximum absolute value of the eigenvalues. Since $M_H(-z_1, -z_2) = -M_H(z_1, z_2)$, we may assume that $\|M_H(z_1, z_2)\|$ is given by the largest eigenvalue. (For q even, the spectrum of $M_H(z_1, z_2)$ is actually symmetric, as shown on p.233 of [CEY90].) The characteristic polynomial of M_H is of the form: $p_{M_H}(x) = \det(M_H - x\mathbf{1}) = \sum_{k=0}^{q} a_k x^k$ where all the a_k's except a_0 are independent of z_1 and z_2, and with $a_q = (-1)^q$, $a_0 = (-1)^{q+1}(z_1^q + z_1^{-q} + z_2^q + z_2^{-q}) + K$, where K is a constant[7] only depending on q. When q is even $p_{M_H}(x)$ is a polynomial with real coefficients and $a_q = 1$, therefore its largest root is attained when $a_0 = (-1)(z_1^q + z_1^{-q} + z_2^q + z_2^{-q}) + K$ is the smallest, i.e. when $z_1 = z_2 = 1$. When q is odd $p_{M_H}(x)$ is a polynomial with real coefficients and $a_q = -1$, therefore its largest root is attained when $a_0 = z_1^q + z_1^{-q} + z_2^q + z_2^{-q} + K$ is the largest, i.e. when $z_1 = z_2 = 1$. □

We now are able to prove Proposition 4:

Proof of Proposition 4. We set $\theta = p/q \in [0, 1]$, $C_k = \cos(2\pi k(p/q))$,

$$M = \begin{pmatrix} 2C_0 & 1 & 0 & \cdots & 0 & 1 \\ 1 & 2C_1 & 1 & \cdots & 0 & 0 \\ 0 & 1 & 2C_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2C_{q-2} & 1 \\ 1 & 0 & 0 & \cdots & 1 & 2C_{q-1} \end{pmatrix}$$

and $\alpha = \|M\|$. By Lemma 3 we have to prove that $\alpha - 2C_1 \le 2(1+\sqrt{2})$. Note that the norm of the first column of M is $\sqrt{6}$ (or $\sqrt{8}$ if $\theta = \frac{1}{2}$), so that $\alpha = \|M\| > 2$. Let $v = (v_0, v_1, \ldots, v_{q-1})$ be an eigenvector of eigenvalue α. Let v_k be the greatest component in absolute value, we may assume that $v_k > 0$ (replacing v by $-v$ if necessary). As $Mv = \alpha v$ we get $v_{k-1} + 2C_k v_k + v_{k+1} = \alpha v_k$ where the indices are taken mod q. As $\alpha > 2$ we have

[7] For q odd one has $K = 0$, see [CEY90, 3.3]. Note that it is claimed there that this formula holds for any q, but computations with $q = 2$ or $q = 4$ show that this is not the case.

$v_{k\pm 1} =: \max(v_{k-1}, v_{k+1}) > 0$ and $2v_{k\pm 1} + 2C_k v_k \geq \alpha v_k$. The same relation for $v_{k\pm 1}$ gives: $2v_k + 2C_{k\pm 1} v_{k\pm 1} \geq \alpha v_{k\pm 1}$. So we get the two inequalities $(\alpha - 2C_k)v_k \leq 2v_{k\pm 1}$, $(\alpha - 2C_{k\pm 1})v_{k\pm 1} \leq 2v_k$ and since by hypothesis everything is positive we can multiply both inequalities and get

$$(\alpha - 2C_k)(\alpha - 2C_{k\pm 1}) \leq 4.$$

Recall that we want to show $\alpha - 2C_1 - 2(1 + \sqrt{2}) \leq 0$. Suppose by contradiction that $\alpha - 2C_1 - 2(1+\sqrt{2}) > 0$, then $d = -\alpha + 2C_1 + 2(1+\sqrt{2}) < 0$ and as $(\alpha + d - 2C_k) > 0$ and $(\alpha + d - 2C_{k\pm 1}) > 0$ we would get

$$(\alpha + d - 2C_k)(\alpha + d - 2C_{k\pm 1}) < (\alpha - 2C_k)(\alpha - 2C_{k\pm 1}) \leq 4,$$

i.e.

$$(2C_1 + 2(1 + \sqrt{2}) - 2C_k)(2C_1 + 2(1 + \sqrt{2}) - 2C_{k\pm 1}) < 4$$

or

$$(1 + \sqrt{2} + \cos(x) - \cos(y))(1 + \sqrt{2} + \cos(x) - \cos(y \pm x)) < 1,$$

where $x = 2\pi p/q$ and $y = 2\pi kp/q$. A rather delicate but straightforward analysis (see Aappendix A) shows that

$$(1 + \sqrt{2} + \cos(x) - \cos(y))(1 + \sqrt{2} + \cos(x) - \cos(y \pm x)) \geq 1 \quad \forall x, y \in [0, 2\pi]$$

giving a contradiction. □

Remarks.

(1) Despite the abundant literature regarding spectra of periodic Jacobi matrices (see [AS82,Moe76] and the references therein), we are not aware of any estimation of spectral radius similar to Proposition 4.

(2) Based on numerical evidence (see Fig. 1), we conjecture that the stronger bound $\|H_\theta\| \leq 2\sqrt{2}$ holds for $\theta \in [\frac{1}{4}, \frac{1}{2}]$ (with equalities at both ends). The Wilkinson–Rammal formula (see [RB90]) shows that the right derivative of $\|H_\theta\|$ at $\frac{1}{4}$ (resp. the left derivative at $\frac{1}{2}$) is negative (resp. positive), so that this bound certainly holds on a neighbourhood of $\frac{1}{4}$ (resp. $\frac{1}{2}$). Note that the bound $\|H_\theta\| \leq 2(1 + \sqrt{2} + \cos 2\pi\theta)$ is better than the obvious bound $\|H_\theta\| \leq 4$ only for $\theta \in [0.317972, \frac{1}{2}]$.

(3) For $\theta = p/q$, set $q = 2m + 1$ if q is odd and $q = 2m + 2$ if q is even. It is proved in Theorem 3.3 of [CEY90] that $H_{p/q}$ has exactly $2m$ gaps in its spectrum, and that each gap has length at least 8^{-q}. Actually the argument on p.233 of [CEY90] shows the following:
- if q is odd, the length of any gap is at least $(2\|H_{p/q}\|)^{-q+2}$;
- if q is even, the length of any gap is at least $2^{-m}\|H_{p/q}\|^{1-2m}$.

So for θ close to $\frac{1}{2}$ and rational, our Proposition 4 gives a substantially better lower bound on the length of gaps in $Sp(H_\theta)$.

See Section 5 below for potential applications of Proposition 4 to combinatorics.

4. Powers of H_θ

Fix $\theta \in [0, 1]$ and set $\rho = e^{2\pi i\theta}$. Any element X in the $C*$-algebra $\mathcal{A}_\theta$ has a "Fourier expansion": $X = \sum_{m,n\in\mathbb{Z}} c_{m,n} U^m V^n$. In particular we have for $k \in \mathbb{N}$, ${H_\theta}^k = \sum_{m,n\in\mathbb{Z}} a_{m,n}^{(k)}(\rho) U^m V^n$ where $a_{m,n}^{(k)}(\rho)$ is a trigonometric polynomial in ρ. We are going to give a combinatorial interpretation of $a_{m,n}^{(k)}(\rho)$. An oriented path in $\mathbb{Z}^2$ will be an oriented polygonal path in $\mathbb{R}^2$, with all vertices and segments contained in the square lattice grid determined by $\mathbb{Z}^2$ in $\mathbb{R}^2$. For $(m, n) \in \mathbb{Z}^2$, denote by $\mathcal{L}_{(m,n)}^{(k)}$ the set of all oriented paths in $\mathbb{Z}^2$, of length k, starting at $(0, 0)$ and ending at (m, n). We also denote by $\gamma_{(m,n)}$ the oriented path in $\mathbb{Z}^2$ with only vertices (m, n), $(m, 0)$ and $(0, 0)$ so that the starting point of $\gamma_{(m,n)}$ is (m, n) while its endpoint is $(0, 0)$. For $\gamma \in \mathcal{L}_{(m,n)}^{(k)}$, we denote by $\gamma \cdot \gamma_{(m,n)}$ the closed path obtained by composing γ with $\gamma_{(m,n)}$, and we denote by $A(\gamma \cdot \gamma_{(m,n)})$ the oriented area enclosed by $\gamma \cdot \gamma_{(m,n)}$, i.e. $A(\gamma \cdot \gamma_{(m,n)}) = \oint_{\gamma\cdot\gamma_{(m,n)}} x\,\mathrm{d}y = -\oint_{\gamma\cdot\gamma_{(m,n)}} y\,\mathrm{d}x$.

Proposition 5.

$$a_{m,n}^{(k)}(\rho) = \sum_{\gamma\in\mathcal{L}_{(m,n)}^{(k)}} \rho^{-A(\gamma\cdot\gamma_{(m,n)})} = \sum_{l\in\mathbb{Z}} \rho^{-l} \#\{\gamma \in \mathcal{L}_{(m,n)}^{(k)}: A(\gamma \cdot \gamma_{(m,n)}) = l\}.$$

Remark. Recall that $\mathcal{A}_\theta$ carries a faithful tracial state τ_θ: for an element $X = \sum_{m,n\in\mathbb{Z}} c_{m,n} U^m V^n$ of $\mathcal{A}_\theta$ one has $\tau_\theta(X) = c_{0,0}$. (For $\theta \notin \mathbb{Q}$, the trace τ_θ is the unique tracial state on $\mathcal{A}_\theta$, see [Rie81] for all these.) The combinatorial interpretation of $\tau_\theta({H_\theta}^k) = a_{0,0}^{(k)}$ is especially appealing: $\mathcal{L}_{(0,0)}^{(k)}$ is the set of closed oriented paths in $\mathbb{Z}^2$, based at $(0, 0)$ and with length k and

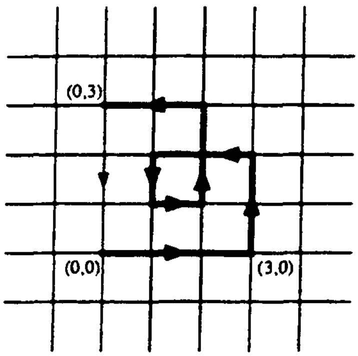
$$\begin{aligned}\tau_\theta({H_\theta}^k) &= \sum_{\gamma\in\mathcal{L}_{(0,0)}^{(k)}} \rho^{-A(\gamma)} \\ &= \#\{\gamma \in \mathcal{L}_{(0,0)}^{(k)}: A(\gamma) = 0\} + \sum_{l\geq 1} \#\{\gamma \in \mathcal{L}_{(0,0)}^{(k)}: A(\gamma) = l\} \cdot 2\cos 2\pi l\theta.\end{aligned}$$

The final formula follows by reordering the first summation according to values of $A(\gamma)$, and noticing that reversing the orientation of paths induces a bijection between $\#\{\gamma \in \mathcal{L}_{(m,n)}^k: A(\gamma) = l\}$ and $\#\{\gamma \in \mathcal{L}_{(m,n)}^k: A(\gamma) = -l\}$. Bellissard and Zelditch informed us that they were aware of this combinatorial interpretation of $\tau_\theta({H_\theta}^k)$.

Proof of Proposition 5. Suppose we expand ${H_\theta}^k = (U_\theta + U_\theta^{-1} + V_\theta + V_\theta^{-1}) \cdots (U_\theta + U_\theta^{-1} + V_\theta + V_\theta^{-1})$ in monomials $U_\theta^{i_1} V_\theta^{j_1} U_\theta^{i_2} V_\theta^{j_2} \cdots$ or $V_\theta^{j_1} U_\theta^{i_1} V_\theta^{j_2} U_\theta^{i_2} \cdots$; one of these monomials will contribute to $a_{m,n}^{(k)}(\rho)$ iff it is of bi-degree (m, n), i.e. $i_1 + i_2 + \cdots = m$

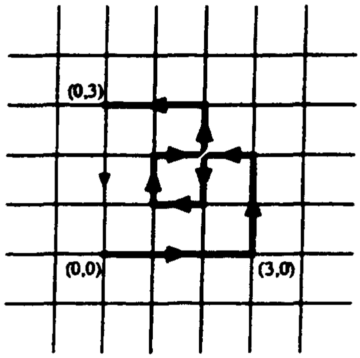
and $j_1 + j_2 + \cdots = n$. To any such monomials $U_\theta^{i_1} V_\theta^{j_1} U_\theta^{i_2} V_\theta^{j_2} \cdots$ we associate a path $\gamma \in \mathcal{L}^k_{(m,n)}$ with vertices $(0,0)$, $(i_1, 0)$, (i_1, j_1), $(i_1 + i_2, j_1)$, $(i_1 + i_2, j_1 + j_2)$,. . .Let us give two examples.

$U_\theta^3 V_\theta^2 U_\theta^{-2} V_\theta^{-1} U_\theta V_\theta^2 U_\theta^{-2}$ gives:



where $A(\gamma \cdot \gamma_{(0,3)}) = 9$,

and $U_\theta^3 V_\theta^2 U_\theta^{-1} V_\theta^{-1} U_\theta^{-1} V_\theta U_\theta V_\theta U_\theta^{-2}$:



where $A(\gamma \cdot \gamma_{(0,3)}) = 7$.

Conversely to any path $\gamma \in \mathcal{L}^k_{(m,n)}$ we associate such a monomial of bi-degree (m, n) in the expansion of H_θ^{2k}. Let us reduce $U_\theta^{i_1} V_\theta^{j_1} U_\theta^{i_2} V_\theta^{j_2} \cdots$ using the commutation relations.

$$\begin{aligned} U_\theta^{i_1} V_\theta^{j_1} U_\theta^{i_2} V_\theta^{j_2} \cdots &= \rho^{i_2 j_1} U_\theta^{i_1+i_2} V_\theta^{j_1+j_2} U_\theta^{i_3} V_\theta^{j_3} \cdots \\ &= \rho^{i_2 j_1 + i_3(j_1+j_2)} U_\theta^{i_1+i_2+i_3} V_\theta^{j_1+j_2+j_3} U_\theta^{i_4} V_\theta^{j_4} \cdots \\ &= \rho^{i_2 j_1 + i_3(j_1+j_2)+i_4(j_1+j_2+j_3)} U_\theta^{i_1+i_2+i_3+i_4} V_\theta^{j_1+j_2+j_3+j_4} U_\theta^{i_5} \cdots \\ &= \cdots \end{aligned}$$

For γ the associated path one computes

$$-A(\gamma \cdot \gamma_{(m,n)}) = \oint\limits_{\gamma \cdot \gamma_{(m,n)}} y \, \mathrm{d}x = i_2 j_1 + i_3(j_1 + j_2) + i_4(j_1 + j_2 + j_3) + \cdots$$

The computation for a monomial $V_\theta^{j_1} U_\theta^{i_1} V_\theta^{j_2} U_\theta^{i_2} \cdots$ is entirely similar. This proves the first equality. To get the second, just reorder the first summation according to values of $A(\gamma \cdot \gamma_{(m,n)})$. □

Let us conclude by giving some properties of the coefficients $a_{m,n}^{(k)}(\rho)$, using the above combinatorial formula and the following lemma :

Lemma 4. *The coefficients $a^{(k)}_{m,n}(\rho)$ satisfy the recursion formulas:*

$$a^{(k)}_{m,n}(\rho) = a^{(k-1)}_{m-1,n}(\rho) + a^{(k-1)}_{m+1,n}(\rho) + a^{(k-1)}_{m,n-1}(\rho)\cdot\rho^{m} + a^{(k-1)}_{m,n+1}(\rho)\cdot\rho^{-m},$$

$$a^{(k)}_{m,n}(\rho) = a^{(k-1)}_{m-1,n}(\rho)\cdot\rho^{n} + a^{(k-1)}_{m+1,n}(\rho)\cdot\rho^{-n} + a^{(k-1)}_{m,n-1}(\rho) + a^{(k-1)}_{m,n+1}(\rho).$$

Proof. Using the commutation relation $V_\theta U_\theta = \rho U_\theta V_\theta$ and the trivial equalities ${H_\theta}^k = H_\theta \cdot {H_\theta}^{k-1}$ and ${H_\theta}^k = {H_\theta}^{k-1}\cdot H_\theta$, the proof is a straightforward computation. □

Then one can easily prove the following result.

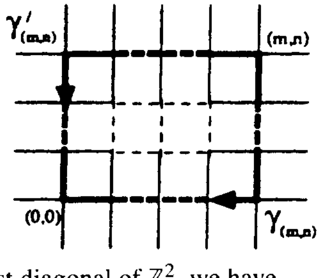
Proposition 6. *For any $m, n \in \mathbb{Z}$, $k \geq 1$:*
(a) $a^{(k)}_{m,n}(\rho) = a^{(k)}_{n,m}(\rho)$,
(b) $a^{(k)}_{m,n}(\rho^{-1}) = a^{(k)}_{m,n}(\rho)\cdot\rho^{-mn}$,
(c) $a^{(k)}_{-m,n}(\rho) = a^{(k)}_{m,n}(\rho^{-1})$ *and* $a^{(k)}_{m,-n}(\rho) = a^{(k)}_{m,n}(\rho^{-1})$.

Proof.
(a) The equality is trivial for $k = 1$, then by induction on k and using Lemma 4 one gets

$$\begin{aligned} a^{(k)}_{m,n}(\rho) &= a^{(k-1)}_{m-1,n}(\rho) + a^{(k-1)}_{m+1,n}(\rho) + a^{(k-1)}_{m,n-1}(\rho)\cdot\rho^{m} + a^{(k-1)}_{m,n+1}(\rho)\cdot\rho^{-m} \\ &= a^{(k-1)}_{n,m-1}(\rho) + a^{(k-1)}_{n,m+1}(\rho) + a^{(k-1)}_{n-1,m}(\rho)\cdot\rho^{m} + a^{(k-1)}_{n+1,m}(\rho)\cdot\rho^{-m} \\ &= a^{(k)}_{n,m}(\rho). \end{aligned}$$

(b) As in (a), the proof is an easy induction on k, using both recursion formulas of Lemma 4.
(c) The symmetry α given by $(x, y) \longmapsto (-x, y)$ induces a bijection between $\mathcal{L}^k_{(m,n)}$ and $\mathcal{L}^k_{(-m,n)}$; moreover $\alpha(\gamma_{(m,n)}) = \gamma_{(-m,n)}$ and $A(\alpha(\gamma)\cdot\gamma_{(-m,n)}) = -A(\gamma\cdot\gamma_{(m,n)})$ for $\gamma \in \mathcal{L}^k_{(m,n)}$; this proves the first relation. The proof of the second is similar. □

Note the following combinatorial consequence of Proposition 6(a). For $(m, n) \in \mathbb{Z}^2$, denote by $\gamma'_{(m,n)}$ the oriented path in $\mathbb{Z}^2$ with origin (m, n), extremity $(0, 0)$ and only intermediate vertex $(0, n)$.



Just by symmetry on the first diagonal of $\mathbb{Z}^2$, we have

$$\#\{\gamma \in \mathcal{L}^{(k)}_{(m,n)}: A(\gamma\cdot\gamma'_{(m,n)}) = l\} = \#\{\gamma \in \mathcal{L}^{(k)}_{(n,m)}: A(\gamma\cdot\gamma_{(n,m)}) = -l\}.$$

Combining Propositions 5 and 6(a), we get

$$\#\{\gamma \in \mathcal{L}^{(k)}_{(m,n)} \colon A(\gamma \cdot \gamma'_{(m,n)}) = l\} = \#\{\gamma \in \mathcal{L}^{(k)}_{(m,n)} \colon A(\gamma \cdot \gamma_{(m,n)}) = -l\}.$$

Remark. Consider again the generating subset $S_0 = \{x, y, x^{-1}, y^{-1}\}$ of $\Gamma = H(\mathbb{Z})$. As in the beginning of Section 2, the adjacency operator of the Cayley graph $\mathcal{G}(\Gamma, S_0)$ is $A_{S_0} = x + x^{-1} + y + y^{-1} \in C^*_r(\Gamma)$. Taking $\rho = e^{2\pi i\theta}$ as an indeterminate, all the above information on powers on H_θ can be lifted up to Γ, to yield results about powers of A_{S_0}. Indeed, viewing the $a^{(k)}_{m,n}$'s as Laurent polynomials in z, one has

$$A^k_{S_0} = \sum_{m,n\in\mathbb{Z}} a^{(k)}_{m,n}(z^{-1}) x^m y^n.$$

In turn, this gives information on the walk-generating function of $\mathcal{G}(\Gamma, S_0)$: for an element $g \in \Gamma$, the associated walk-generating function is the formal power series $W_g(Z) = \sum_{k=0}^{\infty} W^{(k)}_g Z^k$ where $W^{(k)}_g$ is the number of paths of length k from 1 to g in $\mathcal{G}(\Gamma, S_0)$. Clearly $W^{(k)}_g = \langle A^k_{S_0}\delta_1 | \delta_g\rangle$ so that, for $g = z^L x^M y^N$, the coefficient of the term of degree L in the Laurent polynomial $a^{(k)}_{M,N}(z^{-1})$ is precisely $W^{(k)}_g$. See also Lemma 5 below for more on the philosophy of "lifting" from $\mathbb{Z}^2$ to $H(\mathbb{Z})$. We now turn to other bounds on $\|H_\theta\|$.

We already noticed in the final remark of Section 3 that the bound of Proposition 4 is good only in a neighbourhood of $\frac{1}{2}$. On the other hand, it is possible to get bounds that are good except in a neighbourhood of $\frac{1}{2}$, by a mere application of the triangle inequality. Indeed, recall that

$$H_\theta{}^k = \sum_{m,n\in\mathbb{Z}} a^{(k)}_{m,n}(\rho) U^m_\theta V^n_\theta$$

and set

$$g_k(\theta) = \left[\sum_{m,n\in\mathbb{Z}} \left|a^{(k)}_{m,n}(\rho)\right|\right]^{1/k},$$

we then have $\|H_\theta\| \le g_k(\theta)$ for any $\theta \in [0, 1]$ and[8] $k \in \mathbb{N}$. It is experimentally found that, at least for k even, this bound is very good, see Fig. 3.

This can be partially explained by the following result.

Proposition 7.
(a) *For any* $k \in \mathbb{N}$, $\theta \in [0, 1]$, $g_k(\theta) \le g_k(0) = 4$.
(b) *For* k *even*, $g_k(\frac{1}{2}) = 2\sqrt{2}$.

[8] For $k = 2$, this is nothing but the "diamagnetic inequality" $\|H_\theta\| \le 4\cos\frac{1}{2}\pi\theta$ ($\theta \in [0, \frac{1}{2}]$), which seems to be well known to physicists.

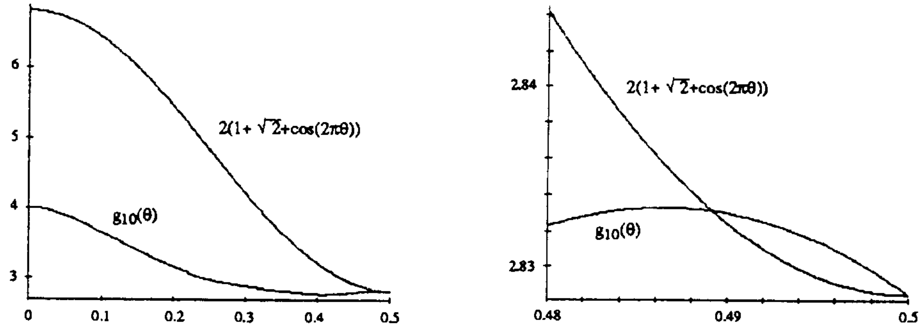


Fig. 3.

Proof.

(a) By Proposition 5, the $a_{m,n}^{(k)}(\rho)$'s are trigonometric polynomials with non-negative coefficients, so that $|a_{m,n}^{(k)}(\rho)| \le a_{m,n}^{(k)}(1)$ and $g_k(\theta) \le \left[\sum_{m,n\in\mathbb{Z}} a_{m,n}^{(k)}(1)\right]^{1/k} = g_k(0)$. Now $\sum_{m,n\in\mathbb{Z}} a_{m,n}^{(k)}(1)$ is just the number of paths of length k in $\mathbb{Z}^2$ with origin $(0,0)$: this number is equal to 4^k.

(b) We begin with:
Claim. Let $\theta = p/q$ be rational. Let $X = \sum_{m,n\in\mathbb{Z}} c_{m,n} U_\theta^m V_\theta^n$ be the Fourier expansion of an element $X \in \mathcal{A}_\theta$ with $c_{m,n} \ge 0$ for any m, n. Assume that there exists integers r, s with q dividing rs such that $X \in C^*(U_\theta^r, V_\theta^s)$, the C^*-subalgebra generated by U_θ^r and V_θ^s (this means that $c_{m,n} = 0$ except if r divides m and s divides n). Then $\|X\| = \sum_{m,n\in\mathbb{Z}} c_{m,n}$. Indeed one has $V_\theta^s U_\theta^r = \rho^{rs} U_\theta^r V_\theta^s = U_\theta^r V_\theta^s$ so that $C^*(U_\theta^r, V_\theta^s)$ is abelian. Let then $\chi: C^*(U_\theta^r, V_\theta^s) \longmapsto \mathbb{C}$ be the trivial character, defined by $\chi(U_\theta^r) = \chi(V_\theta^s) = 1$. By continuity of χ we have $\chi(X) = \sum_{m,n\in\mathbb{Z}} c_{m,n} \le \|X\|$, the reverse inequality is obvious.
To prove Proposition 7(b), we take $\theta = \frac{1}{2}$, $X = H_{1/2}^{2l}$, and we apply the claim with $r = s = 2$: it gives $g_k(\frac{1}{2})^{2l} = \|H_{1/2}^{2l}\| = \|H_{1/2}{}^{2l}\| = (2\sqrt{2})^{2l}$. □

Remarks.

(1) For $\theta = \frac{1}{2}$, the fact that $H_{1/2}^{2l}$ belongs to $C^*(U_\theta^2, V_\theta^2)$ has the following combinatorial consequence: for m, n odd integers, the number of oriented paths γ in $\mathbb{Z}^2$ with origin $(0,0)$, length $2l$, and $A(\gamma \cdot \gamma_{m,n})$ even, is equal to the number of oriented paths γ in $\mathbb{Z}^2$ with same origin, same length, and $A(\gamma \cdot \gamma_{m,n})$ odd. Of course this can also be proved directly.

(2) For $\theta = \frac{1}{4}$, the claim in Proposition 7 applies to $(H_\theta{}^2 - 4)^2$, allowing one to give an upper bound on $\theta \longrightarrow \|H_\theta\|$ that yields the correct value $2\sqrt{2}$ both at $\frac{1}{4}$ and $\frac{1}{2}$, and the correct value 4 at 0.

Finally let us just remark that the tracial state on $\mathcal{A}_\theta$ can be used to get lower bounds on $\|H_\theta\|$. Indeed, it follows from measure theory (see e.g. [HRV93a, Lemma 8]) that, for

Table 1

k	$f_k(\frac{1}{2})$	k	$f_k(\frac{1}{2})$	k	$f_k(\frac{1}{2})$
1	2	10	2.46554511	19	2.586734171
2	2.114742527	11	2.485528971	20	2.594971276
3	2.195514639	12	2.503219974	21	2.602603395
4	2.258100864	13	2.518994081	22	2.609697173
5	2.308804851	14	2.533151187	23	2.616309679
6	2.350888285	15	2.545932671	24	2.622490069
7	2.386373823	16	2.557537987	25	2.628280919
8	2.416664162	17	2.568117362	26	2.633719301
9	2.442792734	18	2.577813758	$\|H_{1/2}\|$	2.828427125

any self-adjoint operator H in $\mathcal{A}_\theta$. $\|H\| = \lim_{k\to\infty} \tau_\theta(H^{2k})^{1/2k}$. We apply this to Harper's operator H_θ.

Proposition 8.
(a) *For any* $k \in \mathbb{N}$, *the function* $f_k: \theta \longmapsto \tau_\theta(H^{2k})^{1/2k}$ *is a* C^∞*-function on* $[0, 1]$.
(b) *For any* $\theta \in [0, 1]$, *the sequence* $(f_k(\theta))_{k\geq 1}$ *increases to* $\|H_\theta\|$.
(c) *The sequence of functions* $(f_k)_{k\geq 1}$ *converges uniformly on* $[0, 1]$ *to* $\theta \longmapsto \|H_\theta\|$.

Proof.
(a) The function $\theta \longmapsto \tau_\theta(H^{2k})$ is a non-negative trigonometrical polynomial.
(b) By Hölder's inequality with $p = (k+1)/k$, $q = k+1$, we have $f_k(\theta)^{2k} = \tau_\theta(H^{2k}) \leq \tau_\theta(H^{2k+2})^{k/(k+1)}\tau_\theta(1)^{1/(k+1)} = f_{k+1}(\theta)^{2k}$.
(c) Since the limit function $\theta \longmapsto \|H_\theta\|$ is continuous [Ell82], this property follows from (b) and Dini's lemma. □

Remark. Numerical calculations show that the convergence of the sequence $(f_k(\theta))_{k\geq 1}$ is very slow. Table 1 illustrates this slowness at the point $\theta = \frac{1}{2}$.

5. Combinatorial applications

Proposition 3 gives the spectrum of the adjacency matrix A on the Cayley graph $\mathcal{G} = \mathcal{G}(H(\mathbb{Z}), S)$; indeed, we have $A = 6h_S$ (since $\mathcal{G}$ is regular of degree 6), hence $Sp(A) = [-2-2\sqrt{2}, 6]$. The combinatorial Laplace Δ operator on $\mathcal{G}$ is related to A by $\Delta = 6\cdot\mathbf{1} - A$, so we also have

$$Sp(\Delta) = [0, 8+2\sqrt{2}].$$

Now $\mathcal{G}$ covers a family $(\mathcal{G}_N)_{N\geq 1}$ of finite, 6-regular graphs obtained as follows: let $H(\mathbb{Z}/N\mathbb{Z})$ be the Heisenberg group over the ring $\mathbb{Z}/N\mathbb{Z}$, i.e.

$$H(\mathbb{Z}/N\mathbb{Z}) = \left\{ \begin{pmatrix} 1 & x & z \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix} : x, y, z \in \mathbb{Z}/N\mathbb{Z} \right\}$$

and let $\alpha_N: H(\mathbb{Z}) \longrightarrow H(\mathbb{Z}/N\mathbb{Z})$ be the reduction modulo N; this is a surjective homomorphism. Now let $\mathcal{G}_N$ be the Cayley graph $\mathcal{G}(H(\mathbb{Z}/N\mathbb{Z}), \alpha_N(S))$: this is a 6-regular graph on N^3 vertices, and we denote by A_N its adjacency matrix. Clearly $Sp(A_N) \subseteq Sp(A) = [-2-2\sqrt{2}, 6]$; moreover, it follows from [Lüc94] that, for $(N_k)_{k\geq 1}$ an increasing sequence of positive integers with $N_k | N_{k+1}$, the spectral measure of A_{N_k} converges weakly, for $k \longmapsto \infty$, to the spectral measure of A. This implies in particular that, for $k \longmapsto \infty$, the lowest eigenvalue $\lambda_{\min}(N_k)$ of A_{N_k} converges to $-2-2\sqrt{2}$.

The independence number $i(X)$ of a finite, k-regular graph X is the maximal number of pairwise non-adjacent vertices in X. It is an unpublished result of Hofmann (see [Hae] for a proof) that

$$\mathrm{i}(X) \leq |X| \frac{1}{1 - k/\lambda_{\min}(X)}.$$

For the graphs $\mathcal{G}_N$, using $k = 6$ and $\lambda_{\min}(X) \geq -2-2\sqrt{2}$, one gets:[9] $\mathrm{i}(\mathcal{G}_N) \leq 0.446 \cdot N^3$

We now turn to applications to asymptotics of closed paths through the origin in the square lattice $\mathbb{Z}^2$. We denote by $N(2k)$ the cardinality of $\mathcal{L}^{2k}_{(0,0)}$, i.e. the number of closed oriented paths through $(0,0)$, of length $2k$ in $\mathbb{Z}^2$. It is well known (see e.g. [DS84, 7.3]) that

$$N(2k) = \sum_{l=0}^{k} \binom{2k}{l, l, k-l, k-l} = \binom{2k}{k}^2.$$

From this, it follows easily (by Stirling's formula) that $\lim_{k\to\infty} N(2k)^{1/2k} = 4$ or, equivalently, that $\log N(2k)$ behaves asymptotically like $2k \log 4$:

$$\log N(2k) \sim 2k \log 4$$

($\sim$ means that the ratio tends to 1 for $k \to \infty$).

Denote by $N(2k;\ A = l)$ the number of paths in $\mathcal{L}^{2k}_{(0,0)}$ with area l; also, denote by $N(2k;\ A \equiv l \pmod q)$ the number of paths in $\mathcal{L}^{2k}_{(0,0)}$ whose area is congruent to l modulo q. Next lemma is that $\log N(2k) \sim \log N(2k;\ A = 0)$. This seems to indicate that, in the decomposition $N(2k) = \sum_l N(2k;\ A = l)$, the term $N(2k;\ A = 0)$ is dominant.

Lemma 5. $\lim_{k\to\infty} N(2k;\ A = 0)^{1/2k} = 4$; *in other words* $\log N(2k;\ A = 0) \sim 2k \log 4$.

Proof. Let $S_0 = \{x, y, x^{-1}, y^{-1}\}$ be the generating subset of $\Gamma = H(\mathbb{Z})$ appearing in Lemma 2. View the Cayley graph $\mathcal{G}(\Gamma, S_0)$ as a covering of the square grid, via the map

[9] For a finite k-regular graph X, there are combinatorial quantities which are known to depend on $\lambda_{\min}(X)$; this is the case of the chromatic number or the number of spanning trees [Big93, 8.8, 6.5]. But for the $\mathcal{G}_N$'s these applications are deceptive: indeed the ratio $k/(-\lambda_{\min}(\mathcal{G}_N)) \approx 6/(2+2\sqrt{2})$ is too close to 1 to be of any use. For example, if $\chi(X)$ is the chromatic number of the finite k-regular graph X, one has $\chi(X) \geq 1 + k/(-\lambda_{\min}(X))$; here $\chi(\mathcal{G}_{\mathcal{N}}) \geq 1 + 6/(2+2\sqrt{2})$ just gives the obvious fact that $\mathcal{G}_{\mathcal{N}}$ is not bipartite.

$\Gamma \longrightarrow \Gamma/Z(\Gamma) \simeq \mathbb{Z}^2$. Viewing Γ as a central extension of $\mathbb{Z}^2$, we may consider the 2-cocycle c on $\mathbb{Z}^2$ giving this central extension: it is

$$c((m_1, n_1), (m_2, n_2)) = \det \begin{vmatrix} m_1 & m_2 \\ n_1 & n_2 \end{vmatrix},$$

which is nothing but the oriented area of the parallelogram on (m_1, n_1) and (m_2, n_2). Let then γ be a closed curve through $(0, 0)$ in $\mathbb{Z}^2$; we lift this curve to a curve $\tilde{\gamma}$ in $\mathcal{G}(\Gamma, S_0)$, starting at the identity. It follows from the above considerations that the endpoint of $\tilde{\gamma}$ will be $z^{A(\gamma)}$. In particular, γ will lift to a closed curve in $\mathcal{G}(\Gamma, S_0)$ if and only if $A(\gamma) = 0$. This shows that $N(2k;\ A = 0)$ is exactly the number of closed curves of length $2k$ through the origin in $\mathcal{G}(\Gamma, S_0)$. Since Γ is amenable and $\mathcal{G}(\Gamma, S_0)$ is a 4-regular graph, we have $\lim_{k\to\infty} N(2k;\ A = 0)^{1/2k} = 4$ by Lemma 2.2 in [Kes59b]. □

Remark. It is also possible to prove this lemma by exploiting Propositions 5 and 8, but the above proof, suggested by E. Ghys, is more conceptual.

Proposition 9. For $\theta = p/q$,

$$\log \left[\sum_{l=0}^{q-1} \mathrm{e}^{-2\pi i l p/q} N(2k;\ A \equiv l \ (\mathrm{mod}\, q)) \right] \sim 2k \log \|H_\theta\|.$$

This follows immediately from Propositions 5 and 8. Note that, by Lemma 5, the term $N(2k;\ A \equiv 0 \ (\mathrm{mod}\, q))$ is "dominant" in the above sum, in the sense that $\log(N(2k;\ A \equiv 0 \ (\mathrm{mod}\, q))) \sim 2k \log 4$. Let us spell out Proposition 9 in the case of some simple fractions:

– for $\theta = \frac{1}{2}$, we have $\|H_\theta\| = 2\sqrt{2}$ and

$$\log(N(2k;\ A \equiv 0 \ (\mathrm{mod}\, 2)) - N(2k;\ A \equiv 1 \ (\mathrm{mod}\, 2))) \sim k \log 8;$$

– for $\theta = \frac{1}{3}$, we have $\|H_\theta\| = 1 + \sqrt{3}$ and

$$\log(N(2k;\ A \equiv 0 \ (\mathrm{mod}\, 3)) - N(2k;\ A \equiv 1 \ (\mathrm{mod}\, 3))) \sim 2k \log(1 + \sqrt{3})$$

(indeed $N(2k;\ A \equiv 1 \ (\mathrm{mod}\, 3)) = N(2k;\ A \equiv -1 \ (\mathrm{mod}\, 3))$);

– for $\theta = \frac{1}{4}$, we have $\|H_\theta\| = 2\sqrt{2}$ and

$$\log(N(2k;\ A \equiv 0 \ (\mathrm{mod}\, 4)) - N(2k;\ A \equiv 2 \ (\mathrm{mod}\, 4))) \sim k \log 8.$$

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Appendix

Lemma A.1. *For any $x, y \in \mathbb{R}$, the two following inequalities hold*:

$$(1+\sqrt{2}+\cos(x)-\cos(y))(1+\sqrt{2}+\cos(x)-\cos(y\pm x)) \geq 1.$$

Proof. Both inequalities are equivalent by the change of variables $x \mapsto -x$. We work with the first one (with a "+"). Using the change of variables $x \mapsto x+\pi$, it is still equivalent to the inequality

$$(1+\sqrt{2}-\cos(x)-\cos(y))(1+\sqrt{2}-\cos(x)+\cos(y+x)) \geq 1$$

that we prove, by restricting to $x, y \in [0, 2\pi]$.

Consider the polynomial $P(t,u) = 4t^4 + t^2(1+4\sqrt{2}) - 2tu(\sqrt{2}+2t^2) + u^2$.

Claim. For $0 \leq t \leq 1$, $u \leq 1$, $P(t,u) \geq 0$

Assume this claim for the moment, the inequality of the claim can be re-written

$$(\sqrt{2}+2t^2)^2 - 2tu(\sqrt{2}+2t^2) + t^2u^2 - (1-t^2)(1-u^2) \geq 1.$$

Setting $t = \sin(\frac{1}{2}x)$, $u = \sin(\frac{1}{2}(x+2y))$ and using standard trigonometric formulas then proves the desired inequality.

To prove the claim, we consider $P_t(u) = P(t,u)$ as a quadratic polynomial in u with parameter t; its discriminant is $t^2[4t^4-(4-4\sqrt{2})t^2+1-4\sqrt{2}]$. The biquadratic polynomial $4t^4-(4-4\sqrt{2})t^2+1-4\sqrt{2}$ has a unique root t^+ in $[0,1]$. So the discriminant is non-positive for $0 \leq t \leq t^+$, which already proves the claim for $0 \leq t \leq t^+$. On the other hand, for $t^+ \leq t \leq 1$, the same biquadratic polynomial increases from 0 to 1, which yields the inequality

$$1+t(1-\sqrt{2}) \geq 1+t[(4t^4-(4-4\sqrt{2})t^2+1-4\sqrt{2})^{1/2}-\sqrt{2}].$$

The left hand side is less than $2t^3$ on $[t^+, 1]$, this leads to the inequality

$$1 \leq (2t^2+\sqrt{2})t - t\sqrt{4t^4-(4-4\sqrt{2})t^2+1-4\sqrt{2}},$$

where the right hand side is nothing but the smallest root of the equation $P_t(u) = P(t,u) = 0$, expressed as a function of t. This shows that for $t^+ \leq t \leq 1$ and $u \leq 1$, one has $P_t(u) = P(t,u) \geq 0$, completing the proof of the claim. □

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