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THE SPECTRUM OF THE ABELIAN SANDPILE MODEL

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Abstract. In their previous work, the authors studied the abelian sandpile model on graphs constructed from a growing piece of a plane or space tiling, given periodic or open boundary conditions, and identified *spectral parameters* which govern the asymptotic spectral gap and asymptotic mixing time. This paper gives a general method of determining the spectral parameters either computationally or asymptotically, and determines the spectral parameters in specific examples.

1. Introduction

When considering Markovian dynamics in a system, important quantities in describing the behavior are the spectral gap, or difference between the largest and second-largest eigenvalue of the transition kernel, and the convergence profile to equilibrium including the mixing time. A central topic in the mixing of large systems is the *cut-off phenomenon*, in which, as the system grows, the transition period to equilibrium is on an asymptotically shorter time scale than the mixing time [9]. In [12] the authors determine theoretically the asymptotic mixing time and prove a cut-off phenomenon for abelian sandpile dynamics on growing pieces of periodic tiling graphs given a periodic or open boundary condition. In [12] it is shown that the spectral gap and asymptotic mixing time are controlled by spectral parameters and spectral factors related to the tiling; these objects are characterized by variational optimization problems. The purpose of this article is to supplement the theoretical results of [12] by demonstrating computational and asymptotic methods of determining the spectral parameters and factors for specific tilings. In doing so, a phenomenon is demonstrated in which a set of open boundary conditions on the D4 lattice in four dimensions causes the asymptotic mixing behavior of the abelian sandpile model to be controlled by the model's behavior along its three-dimensional open boundary.

1.1. **The abelian sandpile model on tiling graphs.** The abelian sandpile model is an important model of self-organized criticality [3], [6], [7], [10], [17],

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[22] which has been studied intensively in the statistical physics literature; see, e.g., survey [18] and the references therein. The model has been studied in various aspects including the effect of the geometry of the underlying graph [2], [8], [15], [19], [21], and the effect of the boundary condition [4], [5], [11], [13], [20]. In [14], Kassel and Wilson calculate a number of statistics for sandpiles on planar periodic tiling graphs, extended here to include the asymptotic spectral gap and asymptotic mixing time. Our results address both the graph geometry and boundary condition.

In sandpile dynamics on a graph $G = (V, E)$ with sink $s \in V$, an allocation of sand $\sigma : V\backslash\{s\} \to \mathbb{Z}_{\geqslant 0}$ gives a state of the model. A state σ is stable if $\sigma(v) < \deg(v)$ for all v, otherwise unstable. If $\sigma(v) \geqslant \deg(v)$ for some v, the node v can topple, passing one grain of sand to each of its neighbors. The dynamics in the model occur in discrete time steps and are Markovian. In each step, a grain of sand is added to the model at a uniform random vertex and all topplings are performed until the model reaches a stable state. The set of recurrent states for the dynamics forms the *sandpile group* $\mathscr{G}$, which is an abelian group isomorphic to $\mathbb{Z}^{V\backslash\{s\}}/\Delta'\mathbb{Z}^{V\backslash\{s\}}$, where Δ' is the reduced graph Laplacian; see [12]. Restricted to recurrent states, the dynamics become a random walk on $\mathscr{G}$, driven by the probability measure

$$\mu = \frac{1}{|V|}\left(\delta_0 + \sum_{v \in V\backslash\{s\}} \delta_{e_v}\right),$$

where e_v is the standard basis vector corresponding to v. The eigenvalues of these dynamics are given by the Fourier coefficients of μ in the dual group, and the *spectral gap* is the difference between 1 and the magnitude of the second-largest eigenvalue. The *total variation mixing time* to uniformity is

$$t^{\mathrm{mix}} = \min_n \|\mu^{*n} - \mathbb{U}_{\mathscr{G}}\|_{\mathrm{TV}} < \frac{1}{e},$$

where $\mathbb{U}_{\mathscr{G}}$ denotes the uniform probability measure on $\mathscr{G}$.

A periodic plane or space tiling in $\mathbb{R}^d$ is an undirected, connected, straight-line edge graph $\mathscr{T}$ which is periodic in a lattice Λ in $\mathbb{R}^d$ such that $\mathscr{T}/\Lambda$ is finite. In [12], sandpile dynamics are considered on two types of graphs constructed from a growing piece of a periodic plane or space tiling. Let $m \geqslant 1$ be an integer.

(I) Assume $\mathscr{T}$ is embedded in $\mathbb{R}^d$ with a vertex at 0. The *periodic boundary graph* is $\mathbb{T}_m = \mathscr{T}/m\Lambda$ with 0 designated sink.

(II) Denote the coordinate hyperplanes $H_{i,j} = \{x \in \mathbb{R}^d : x_i = j\}$. If $\mathscr{T}$ has reflection symmetry in the family of coordinate hyperplanes $\{H_{i,j} : 1 \leqslant i \leqslant d, j \in \mathbb{Z}\}$ with no edge of $\mathscr{T}$ crossing a coordinate hyperplane, then the *open boundary graph* $\mathscr{T}_m$ is obtained by quotienting $\mathscr{T}$ by $\{H_{i,mj}, 1 \leqslant i \leqslant d, j \in \mathbb{Z}\}$ and identifying all vertices on the bounding hyperplanes as sink.

Denote Δ the graph Laplacian,

$$\Delta h(v) = \deg(v)h(v) - \sum_{(v,w)\in E} h(w).$$

Given a function $h \in \ell^2(\mathscr{T})$, say that h is *harmonic modulo 1* if $\Delta h \equiv 0 \bmod 1$ and denote the set of such functions $\mathscr{H}^2(\mathscr{T})$. Let $C^1(\mathscr{T})$ denote the set of integer-valued functions on $\mathscr{T}$ which are finitely supported and have sum 0. In [12] the *periodic boundary spectral parameter* of a periodic tiling is defined to be

$$\gamma = \inf \left\{ \sum_{x\in\mathscr{T}} 1 - \cos(2\pi\xi_x) : \Delta\xi \in C^1(\mathscr{T}), \xi \not\equiv 0 \bmod 1 \right\}. \tag{1}$$

For those $\mathscr{T}$ which have reflection symmetry in the coordinate hyperplanes, given a set $S \subset \{1, 2, \dots, d\}$, let $\mathfrak{S}_S$ be the group generated by reflections in the hyperplanes $\{H_{j,0}, j \in S\}$, and let $\mathscr{A}_S(\mathscr{T})$ be functions which are antisymmetric under reflection in each plane $H_{j,0}, j \in S$. Let $\mathscr{H}^2_S(\mathscr{T})$ denote those ℓ^2 harmonic modulo 1 functions in $\mathscr{A}_S(\mathscr{T})$. Again, for $0 \leqslant i < d$ define the *open boundary spectral parameters*[1]

$$\gamma_i = \inf_{\substack{S\subset\{1,2,\dots,d\}\\ |S|=i}} \inf_{\substack{\xi\in\mathscr{H}^2_S(\mathscr{T})\\ \xi\not\equiv 0 \bmod 1}} \sum_{x\in\mathscr{T}/\mathfrak{S}_S} 1 - \cos(2\pi\xi_x). \tag{2}$$

In dimension $d \geqslant 2$ define the ith *spectral factor*

$$\Gamma_i = \frac{d-i}{\gamma_i} \tag{3}$$

and $\Gamma = \max_i \Gamma_i$.

For sandpile dynamics on periodic tiling graphs, the relationship between the spectral parameters of the tiling and the sandpile dynamics is explained in the following two theorems.

Theorem ([12], Theorem 2)**.** *Given a tiling $\mathscr{T}$, as $m \to \infty$, the spectral gap of the transition kernel of sandpile dynamics on $\mathbb{T}_m$ satisfies*

$$\mathrm{gap}_{\mathbb{T}_m} = (1 + o(1))\frac{\gamma}{|\mathbb{T}_m|}. \tag{4}$$

If $\mathscr{T}$ has reflection symmetry in the coordinate hyperplanes with no edges that cross a hyperplane, then the spectral gap of the transition kernel of sandpile dynamics on $\mathscr{T}_m$ satisfies

$$\mathrm{gap}_{\mathscr{T}_m} = (1 + o(1))\frac{\min(\gamma_j : j \geqslant 0)}{|\mathscr{T}_m|}. \tag{5}$$

In particular, the spectral parameters determine the asymptotic spectral gap with either periodic or open boundary condition.

Theorem ([12], Theorem 3)**.** *For a fixed tiling $\mathscr{T}$ in $\mathbb{R}^d$, sandpiles started from a recurrent state on $\mathbb{T}_m$ have asymptotic total variation mixing time*

$$t_{\mathrm{mix}}(\mathbb{T}_m) \sim \frac{\Gamma_0}{2}|\mathbb{T}_m| \log m \tag{6}$$

with a cut-off phenomenon as $m \to \infty$.

If the tiling $\mathscr{T}$ satisfies the reflection condition, then sandpile dynamics started from a recurrent configuration on $\mathscr{T}_m$ have total variation mixing time

$$t_{\mathrm{mix}}(\mathscr{T}_m) \sim \frac{\Gamma}{2}|\mathscr{T}_m| \log m \tag{7}$$

with a cut-off phenomenon as $m \to \infty$.

[1]Note that, in the definition of $\mathscr{H}^2_S(\mathscr{T})$, $\Delta\xi$ is not required to be in $C^1(\mathscr{T})$, so that the definitions of γ and γ_0 differ, although the two notions are shown in [12] to coincide in dimensions at most 4.

Thus the spectral factors determine the asymptotic mixing time.

If $\Gamma = \Gamma_0$ we say that the *bulk* or *top-dimensional behavior* controls the total variation mixing time, and otherwise that the *boundary behavior* controls the total variation mixing time. In [12] it is shown that for two-dimensional tilings satisfying a reflection condition, the bulk behavior always controls the mixing time.

1.2. **Precise statement of results.** Our first result computes the periodic boundary spectral parameter for the triangular (tri) and honeycomb (hex) tilings in two dimensions and the face centered cubic (fcc) tiling in three dimensions. In particular, this determines the asymptotic spectral gap of dynamics for these tilings, and the asymptotic mixing time when the tilings are given periodic boundary condition.

Theorem 1. *The triangular, honeycomb, and face centered cubic tilings have periodic boundary spectral parameters*[2]

$$\begin{aligned}\gamma_{\text{tri}} &= 1.69416(6),\\ \gamma_{\text{hex}} &= 5.977657(7),\\ \gamma_{\text{fcc}} &= 0.3623(9).\end{aligned}$$

Our remaining results concern spectral factors which govern the mixing time of sandpile dynamics on graphs with open boundary condition.

The D4 lattice has vertices $\mathbb{Z}^4 \cup \mathbb{Z}^4 + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and 24 nearest neighbors of 0,

$$U_4 = \{\pm e_1, \pm e_2, \pm e_3, \pm e_4\} \cup \left\{ \frac{1}{2}(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4), \epsilon_i \in \{\pm 1\} \right\}, \tag{8}$$

which have unit Euclidean length. Let the tiling graph have nearest neighbor edges. The elements of the D4 lattice are frequently identified with the "Hurwitz quaternion algebra" in which U_4 is the group of units. Let

$$v_1 = (1,1,0,0),\ v_2 = (1,-1,0,0),\ v_3 = (0,0,1,1),\ v_4 = (0,0,1,-1),$$

and define hyperplanes

$$\mathscr{P}_j = \{x \in \mathbb{R}^4 : \langle x, v_j\rangle = 0\}.$$

The D4 lattice has reflection symmetry in the family of hyperplanes

$$\mathscr{F}_{\text{D4}} = \{nv_j + \mathscr{P}_j : j \in \{1,2,3,4\}, n \in \mathbb{Z}\}, \tag{9}$$

which can be dilated and rotated to correspond with $\{H_{i,j}\}$, and one can check that no nearest neighbor edge in D4 crosses this family of hyperplanes; see [12]. Our next result determines the boundary spectral parameters and spectral factors for the D4 lattice.

Theorem 2. *The spectral parameters of the* D4 *lattice with reflection planes* $\mathscr{F}_{\text{D4}}$ *and open boundary condition are (ϑ denotes a parameter bounded by* 1 *in size)*

$$\begin{aligned}\gamma_{\text{D4},0} &= 0.075554 + \vartheta 0.00024,\\ \gamma_{\text{D4},1} &= 0.0440957 + \vartheta 0.00017,\\ \gamma_{\text{D4},2} &= 0.0389569 + \vartheta 0.00013,\\ \gamma_{\text{D4},3} &= 0.036873324 + \vartheta 0.00012,\\ \gamma_{\text{D4},4} &= 0.0357604 + \vartheta 0.00011.\end{aligned}$$

[2]The digit in parenthesis indicates the last significant digit.

The spectral factors are given by

$$\Gamma_{\mathrm{D4},0} = 52.9428 + \vartheta 0.17,$$
$$\Gamma_{\mathrm{D4},1} = 68.03486 + \vartheta 0.27,$$
$$\Gamma_{\mathrm{D4},2} = 51.3393 + \vartheta 0.17,$$
$$\Gamma_{\mathrm{D4},3} = 27.1201 + \vartheta 0.084.$$

In particular, the total variation mixing time of the dynamics on the D4 *lattice is dominated by the three-dimensional boundary behavior.*

Our final result asymptotically determines the spectral parameters and spectral factors for $\mathbb{Z}^d$ with nearest neighbor edges and with coordinate hyperplanes as reflecting hyperplanes.

Theorem 3. *As $d \to \infty$, the periodic boundary spectral parameter of the $\mathbb{Z}^d$ lattice is*

$$\gamma_{\mathbb{Z}^d} = \frac{\pi^2}{d^2}\left(1 + \frac{1}{2d} + O\left(d^{-2}\right)\right), \tag{10}$$

and the parameters with open boundary condition are

$$\gamma_{\mathbb{Z}^d,j} = \frac{\pi^2}{2d^2}\left(1 + \frac{3}{2d} + O_j\left(d^{-2}\right)\right) \tag{11}$$

and, uniformly in j,

$$\gamma_{\mathbb{Z}^d,j} \geqslant \frac{\pi^2}{2d^2 + d}. \tag{12}$$

For each fixed j,

$$\Gamma_j = \frac{2d^3 - (2j+3)d^2 + O_j(d)}{\pi^2}. \tag{13}$$

In particular, for all d sufficiently large, the total variation mixing time on $\mathbb{Z}^d$ is dominated by the bulk behavior and $\Gamma = \frac{2d^3}{\pi^2}\left(1 - \frac{3}{2d} + O\left(d^{-2}\right)\right)$.

Note that, for all d sufficiently large, $\gamma_{\mathbb{Z}^d} \neq \gamma_{\mathbb{Z}^d,0}$, so that, in the periodic case, the constant $\gamma_{\mathbb{Z}^d}$ which determines the asymptotic spectral gap is not related to the spectral factor Γ_0 which controls the asymptotic mixing time.

1.3. **Discussion of method.** The harmonic modulo 1 functions considered in this article are evaluated only as functions with values in $\mathbb{R}/\mathbb{Z}$, and hence may be assigned values in $\left(-\frac{1}{2}, \frac{1}{2}\right]$. On this interval there are constants $C_1, C_2 > 0$ such that $C_1 x^2 \leqslant 1 - \cos(2\pi x) \leqslant C_2 x^2$. In particular, each ξ considered in the definitions of the spectral factors may be treated as a function in $\ell^2(\mathscr{T})$.

Rather than work with ξ, it is more convenient to work with its prevector $\nu = \Delta\xi$, which is integer valued, and hence behaves discretely. The function ξ is recovered from ν by convolution with the Green's function g on $\mathscr{T}$, $\xi = g * \nu$. Since Δ is bounded from $\ell^2 \to \ell^2$, only prevectors with bounded ℓ^1-norm need be considered, and, in fact, the arguments of [12] reduce the determination of the spectral factors to within a prescribed tolerance to a finite calculation.

Given a prevector ν and a set $S \subset \mathscr{T}$, the value

$$f_S(\xi) = \sum_{x \in S} 1 - \cos(2\pi \xi_x)$$

may be estimated from below by constrained minimization programs. Since the map $\Delta\xi = \nu$ is linear in ξ, the constraints are linear. The objective function f_S is not convex, but $1 - \cos(2\pi\xi_x)$ is convex in the critical region $\left[-\frac{1}{4}, \frac{1}{4}\right]$ and may be approximated piecewise linearly from below outside this region. Enforcing the constraint $\Delta\xi = \nu$ at only finitely many vertices gives a rapid method of obtaining a lower bound for the value of each ξ. Since the linear constraints involve only the neighbors of the vertex at which the constraint is applied, groups of vertices which are two-separated may be treated additively. This reduces to a connected component analysis of the prevector ν. Boundedly many configurations are found to have a sufficiently small value, and then all ways of gluing these candidates together are considered.

To calculate the value of the spectral parameters, a Fourier representation for the Green's function is used. A general recipe for giving this Fourier representation for the Green's function of any tiling is given in [12], and this recipe is used in the specific examples considered here.

2. Notation list

The following list contains the notation used in this paper.

- meas denotes the usual Lebesgue measure on Euclidean space.
- $B_r(x)$ denotes the Euclidean ball of radius r centered at x in $\mathbb{R}^d$. Its measure is $\mathrm{vol}(B_r(x)) = \frac{r^d \pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2}+1)}$.
- The trigonometric functions are abbreviated $e(x) = e^{2\pi i x}$, $c(x) = \cos(2\pi x)$, and $s(x) = \sin(2\pi x)$.
- $\mathscr{T}$ denotes a periodic tiling graph embedded as an undirected graph in Euclidean space of dimension d. The graph is assumed connected with straight line edges. The graph is periodic in a d-dimensional lattice, which is denoted Λ, and the quotient $\mathscr{T}/\Lambda$ is finite.
- Given a set S and a function $\xi : S \to \mathbb{R}/\mathbb{Z}$,
$$f_S(\xi) = \sum_{s \in S} 1 - c(\xi_s).$$
If $S = \mathscr{T}$ the subscript is dropped.
- Given two nodes x, y in a connected graph G, $d(x, y)$ denotes their graph distance. Given a node x and a set of nodes S, $d(x, S) = \inf_{y \in S} d(x, y)$ is the distance of x from the set S.
- Given $x \in \Lambda$, τ_x denotes the translation of functions in $\mathscr{T}$ by x.
- The ℓ^p spaces on a set S are functions $\nu : S \to \mathbb{R}$, $\|\nu\|_p^p = \sum_{t \in S} |\nu(t)|^p$. The ℓ^∞-norm is the sup norm. When the set is not clear from the context, the notation $\|\cdot\|_{p,S}$ is used.
- The spaces $C^\rho(\mathscr{T})$, $\rho = 0, 1, 2$, are integer-valued functions defined so that C^0-functions have bounded support, $C^1(\mathscr{T})$-functions are those C^0-functions of zero sum, and $C^2(\mathscr{T})$ are those C^1 functions of zero moment. The moment of a function is defined by stopping a simple random walk on the period lattice Λ as explained in the next section.
- Given an integer $m \geqslant 1$, $\mathbb{T}_m$ denotes the periodic boundary graph $\mathscr{T}/m\Lambda$. In this case we assume $0 \in \mathscr{T}$ and designate 0 sink in $\mathbb{T}_m$.

- Given an integer $m \geqslant 1$, if after translation $\mathscr{T}$ has reflection symmetry in the coordinate hyperplanes $H_{i,j} = \{x \in \mathbb{R}^d : x_i = j\}$ without edges crossing the hyperplanes, then $\mathscr{T}_m$ denotes the open boundary graph modulo reflection in the planes $H_{i,mj}$ with nodes on the hyperplanes identified as sink.
- All of the asymptotic notation in the paper holds as $m \to \infty$. The notation $h \ll g$ has the same meaning as $h = O(g)$, while, for positive quantities, $h \sim g$ means $\frac{h}{g}$ tends to 1.
- An abelian sandpile on a finite connected graph $G = (V, E)$ with sink s is a function $\sigma : V\backslash\{s\} \to \mathbb{Z}_{\geqslant 0}$. The sandpile group $\mathscr{G}$ consists of all those states σ which are recurrent for sandpile dynamics on G.
- Δ denotes the graph Laplacian on a graph G. Given a function ν on G, $\Delta\nu(v) = \sum_{(v,w)\in E} \nu(v) - \nu(w)$.
- Given $v \in \mathscr{T}$, g_v denotes the Green's function started at v, which satisfies $\Delta g_v = \delta_v$, where δ_v is the Kronecker delta function at v. Given a real-valued function ν, the notation $g * \nu = g_\nu = \sum_v \nu(v) g_v$ is used.
- $Y_{v,j}$ denotes the jth step of random walk started at a node v in a graph G. The transitions of the random walk at a point w choose a uniform random edge from w to traverse.
- T_v is a stopping time for simple random walk started at a node v.
- The space $\mathscr{H}^2(\mathscr{T})$ denotes those harmonic modulo 1 functions $h \in \ell^2(\mathscr{T})$ such that $\Delta h \equiv 0 \bmod 1$. Given a set $S \subset \{1, 2, \ldots, d\}$, $\mathfrak{S}_S$ denotes the reflection group generated by reflections in $H_{i,0}, i \in S$, and $\mathscr{A}_S$ denotes functions on $\mathscr{T}$ which are antisymmetric in the hyperplane $H_{i,0}$ for all $i \in S$. The space $\mathscr{H}^2_S = \mathscr{H}^2 \cap \mathscr{A}_S$ consists of harmonic modulo 1 functions which are antisymmetric in the hyperplanes indexed by S.
- γ denotes the periodic boundary spectral parameter of $\mathscr{T}$, and γ_j denotes the codimension j open boundary spectral parameter of $\mathscr{T}$. $\Gamma_j = \frac{d-j}{\gamma_j}$ is the jth spectral factor, and the spectral factor of $\mathscr{T}$ is $\Gamma = \max_j \Gamma_j$.
- Given a set $S \subset \mathscr{T}$ and a function $\nu : S \to \mathbb{Z}$, the programs
$$P(S, \nu), P'(S, \nu), P_j(S, \nu), Q(S, \nu), Q'(S, \nu), Q_j(S, \nu)$$
denote not necessarily convex optimization programs which have linear constraints.

3. The Green's function of a tiling

Throughout, $\mathscr{T} \subset \mathbb{R}^d$ is a periodic tiling, which is periodic in a lattice Λ contained in $\mathbb{R}^d$, with $\mathscr{T}/\Lambda$ finite. After translation, assume that $0 \in \mathscr{T}$, which is true of all the tilings considered in this article. Given a tiling $\mathscr{T}$ and a vertex v, the Green's function of $\mathscr{T}$ satisfies $\Delta g_v = \delta_v$, where δ_v is the Kronecker delta function at v. The purpose of this section is to give a more complete description of the tilings considered, and to develop their Green's functions.

We indicate a random walk started from v in $\mathscr{T}$ by $Y_{v,0} = v, Y_{v,1}, Y_{v,2}, \ldots$, in which the walker crosses each edge from a given vertex with equal probability. A *stopping time* adapted to the random walk is a random variable N taking values in $\mathbb{Z}_{\geqslant 0} \cup \{\infty\}$ such that the event $\{N = n\}$ is measurable in the sigma algebra $\sigma(\{Y_{v,0}, Y_{v,1}, \ldots, Y_{v,n}\})$. Let T_v be a stopping time for a simple random walk starting at v in $\mathscr{T}$ and stopping at the first positive time that it reaches Λ. This is the same stopping time as the first positive visit to 0 on the finite state Markov chain given by a random walk on $\mathscr{T}/\Lambda$, and hence $\mathbf{Prob}(T_v > n) = O\left(e^{-cn}\right)$ for some constant $c > 0$. See, e.g., [16] for an introduction to finite state Markov chains and stopping times.

In [12] function spaces are defined on $\mathscr{T}$,

$$C^0(\mathscr{T}) = \{h : \mathscr{T} \to \mathbb{Z}, \|h\|_1 < \infty\},$$
$$C^1(\mathscr{T}) = \left\{h \in C^0(\mathscr{T}), \sum_{x\in\mathscr{T}} h(x) = 0\right\},$$
$$C^2(\mathscr{T}) = \left\{h \in C^1(\mathscr{T}), \sum_{x\in\mathscr{T}} h(x)\mathbf{E}[Y_{x,T_x}] = 0\right\}.$$

The convolution of the Green's function g on $\mathscr{T}$ with a function η of bounded support in $\mathscr{T}$ is defined to be

$$g * \eta = g_\eta = \sum_{v\in\mathscr{T}} \eta(v) g_v.$$

In Theorem 7 of [12] it is shown that for $\eta \in C^0(\mathscr{T})$, $g_\eta \in \ell^2(\mathscr{T})$ if and only if $\eta \in C^\rho(\mathscr{T})$ for

$$\rho = \begin{cases} 2 & d = 2, \\ 1 & d = 3, 4, \\ 0 & d \geqslant 5. \end{cases}$$

Also, a characterization of the spectral parameters is given. Let $\mathscr{I} = \{\Delta\eta : \eta \in C^0(\mathscr{T})\}$, and for $\xi : \mathscr{T} \to \mathbb{R}/\mathbb{Z}$,

$$f(\xi) = \sum_{x\in\mathscr{T}} 1 - c(\xi_x).$$

Similarly, given a set S and $\xi : S \to \mathbb{R}/\mathbb{Z}$, define

$$f_S(\xi) = \sum_{x\in S} 1 - c(\xi_x).$$

Recall that given a collection of hyperplanes $\{H_{j,0}, j \in S\}$, $\mathscr{A}_S(\mathscr{T})$ consists of those functions which are antisymmetric in each hyperplane.

Lemma 4. *The spectral parameter γ has characterization; in dimension 2,*

$$\gamma = \{f(g * \nu) : \nu \in C^2(\mathscr{T}) \backslash \mathscr{I}\},$$

and in dimension at least 3,

$$\gamma = \{f(g * \nu) : \nu \in C^1(\mathscr{T}) \backslash \mathscr{I}\}.$$

The parameter γ_j has characterization

$$\gamma_j = \inf_{S\subset\{1,2,\ldots,d\}, |S|=j} \{f_{\mathscr{T}/\mathfrak{S}_S}(g * \nu) : \nu \in C^\rho(\mathscr{T}) \cap \mathscr{A}_S(\mathscr{T}) \backslash \mathscr{I}\}.$$

Proof. See the proof of Lemma 21 in [12]; this follows from the fact that $\xi \in \mathscr{H}^2(\mathscr{T})$ with $\Delta\xi = \nu$ is given by the convolution $\xi = g_\nu$. $\square$

In this article, the above lemma is used to describe the minimization of the spectral parameter as a search problem over integer-valued vectors which are thus discretely distributed.

Let μ be the probability distribution of Y_{0,T_0} on Λ. The following evaluation of the Green's function of a tiling is given in [12].

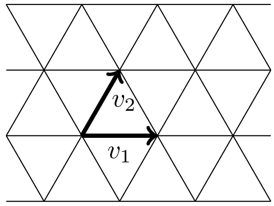

FIGURE 1. The triangular lattice is spanned by vectors v_1, v_2.

Lemma 5. *In dimension 2, for $x \in \Lambda$,*

$$g_0(x) = \sum_{n=0}^{\infty} \frac{\mu^{*n}(x)}{\deg x} - \frac{\mu^{*n}(0)}{\deg 0}, \tag{14}$$

while in dimension $\geqslant 3$,

$$g_0(x) = \sum_{n=0}^{\infty} \frac{\mu^{*n}(x)}{\deg x}, \tag{15}$$

and both sums converge. For $x \notin \Lambda$,

$$g_0(x) = \mathbf{E}[g_0(Y_{x,T_x})]. \tag{16}$$

For $v \notin \Lambda$,

$$g_v(x) = \frac{1}{\deg x}\mathbf{E}\left[\sum_{j=0}^{T_v-1} \mathbf{1}(Y_{v,j} = x)\right] + \mathbf{E}\left[g_{Y_{v,T_v}}(x)\right]. \tag{17}$$

In dimension 2, $g_v(x) \ll 1 + \log(2 + d(v,x))$, and in dimension $d > 2$, $g_v(x) \ll \frac{1}{(1+d(v,x))^{d-2}}$. If $j = 1$ or 2 and $\eta \in C^j(\mathscr{T})$,

$$g_\eta(x) \ll \frac{1}{1 + d(x,0)^{j+d-2}}$$

as $d(x,0) \to \infty$.

Using this lemma the following explicit evaluations are obtained for several lattice tilings. These are used for numerical computations.

3.1. **Triangular lattice (see Figure 1).** This is a lattice, so the Green's function may be calculated without appealing to the stopping time argument above. Let $v_1 = (1,0)$, and let $v_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$. The lattice points take the form $n_1 v_1 + n_2 v_2$ with $n_1, n_2 \in \mathbb{Z}$. The lattice graph is regular of degree 6 and the nearest neighbors to 0 are $\{\pm v_1, \pm v_2, \pm(v_1 - v_2)\}$. Let μ be the measure

$$\mu = \frac{1}{6}\left(\delta_{v_1} + \delta_{-v_1} + \delta_{v_2} + \delta_{-v_2} + \delta_{v_1-v_2} + \delta_{v_2-v_1}\right). \tag{18}$$

The Green's function from 0 is

$$g_0(n_1v_1 + n_2v_2) = \frac{1}{6}\sum_{n=0}^{\infty} \mu^{*n}(n_1v_1 + n_2v_2) - \mu^{*n}(0). \tag{19}$$

This can be obtained via inverse Fourier transform by

$$g_0(n_1v_1 + n_2v_2) = \frac{1}{6}\int_{\mathbb{R}^2/\mathbb{Z}^2} \frac{e(n_1x_1 + n_2x_2) - 1}{1 - \frac{1}{3}\left(c(x_1) + c(x_2) + c(x_1 - x_2)\right)} dx_1 dx_2. \tag{20}$$

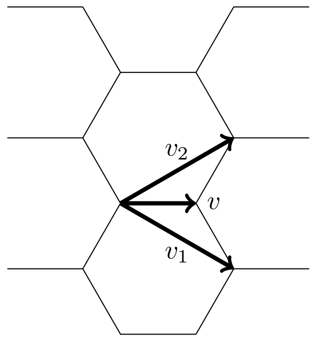

FIGURE 2. Coordinates in the honeycomb tiling are given in terms of the basis for the triangular lattice, v_1, v_2, and $v = \frac{1}{3}(v_1 + v_2)$.

3.2. **Honeycomb tiling (see Figure 2).** This can be constructed from the triangular lattice as follows. Let $v = \frac{1}{3}(v_1 + v_2)$, which is the centroid of the equilateral triangle with vertices at $\{0, v_1, v_2\}$.

The vertices in the tiling have the form $n_1v_1 + n_2v_2$ and $n_1v_1 + n_2v_2 + v$ with $n_1, n_2 \in \mathbb{Z}$. This is a 3-regular graph. The neighbors of a point $n_1v_1+n_2v_2$ are given by $n_1v_1 + n_2v_2 + \{v, -v_1 + v, -v_2 + v\}$. The neighbors of a point $n_1v_1 + n_2v_2 + v$ are $n_1v_1 + n_2v_2 + v + \{-v, -v + v_1, -v + v_2\}$. The tiling has reflection symmetry in the lines in the directions of $v, -v_1 + v, -v_2 + v$ and their translates in the triangular lattice. The random walk started from 0 stops always on the triangular lattice in two steps, so the stopped measure is

$$\mu = \frac{1}{3}\delta_0 + \frac{1}{9}\left(\delta_{v_1} + \delta_{-v_1} + \delta_{v_2} + \delta_{-v_2} + \delta_{v_1-v_2} + \delta_{v_2-v_1}\right). \tag{21}$$

The Green's function started from 0 is given on the triangular lattice by

$$g_0(n_1v_1 + n_2v_2) = \frac{1}{3}\sum_{n=0}^{\infty} \mu^{*n}(n_1v_1 + n_2v_2) - \mu^{*n}(0), \tag{22}$$

which has the integral representation

$$g_0(n_1v_1 + n_2v_2) = \frac{1}{3}\int_{\mathbb{R}^2/\mathbb{Z}^2} \frac{e(n_1x_1 + n_2x_2) - 1}{\frac{2}{3} - \frac{2}{9}\left(c(x_1) + c(x_2) + c(x_1 - x_2)\right)} dx_1 dx_2. \tag{23}$$

By harmonicity,

$$\begin{aligned} g_0(n_1v_1 + n_2v_2 + v) = \frac{1}{3}(&g_0(n_1v_1 + n_2v_2) + g_0((n_1 + 1)v_1 + n_2v_2) \\ &+ g_0(n_1v_1 + (n_2 + 1)v_2)). \end{aligned}$$

By symmetry,

$$g_v(n_1v_1 + n_2v_2 + v) = g_0(n_1v_1 + n_2v_2). \tag{24}$$

Again by harmonicity,

$$\begin{aligned} g_v(n_1v_1 + n_2v_2) = \frac{1}{3}(&g_0(n_1v_1 + n_2v_2) + g_0((n_1 - 1)v_1 + n_2v_2) \\ &+ g_0(n_1v_1 + (n_2 - 1)v_2)). \end{aligned}$$

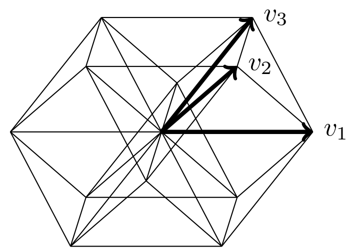

FIGURE 3. Coordinates in the face centered cubic lattice are given in terms of the vectors v_1, v_2, v_3. Any two of these span the triangular lattice.

3.3. **Face centered cubic lattice (see Figure 3).** This is a lattice tiling in $\mathbb{R}^3$ generated by the vectors

$$v_1 = (1,0,0), \qquad v_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right), \qquad v_3 = \left(\frac{1}{2}, \frac{\sqrt{3}}{6}, \frac{\sqrt{6}}{3}\right), \tag{25}$$

which are the vertices of a regular tetrahedron. The tiling graph is regular of degree 12. The neighbors of 0 are

$$\{\pm v_1, \pm v_2, \pm v_3, \pm(v_1 - v_2), \pm(v_1 - v_3), \pm(v_2 - v_3)\}. \tag{26}$$

Let μ be the measure which is uniform on these points. The Green's function started from 0 is given by

$$g_0(n_1v_1 + n_2v_2 + n_3v_3) = \frac{1}{12}\sum_{n=0}^{\infty} \mu^{*n}(n_1v_1 + n_2v_2 + n_3v_3).$$

The Fourier transform is

$$\hat{g}(x_1, x_2, x_3) = \frac{1}{12 - 2(c(x_1) + c(x_2) + c(x_3) + c(x_1 - x_2) + c(x_1 - x_3) + c(x_2 - x_3))}.$$

3.4. D4 **lattice.** The D4 lattice is a lattice in $\mathbb{R}^4$ which is frequently presented as the integer quaternion ring

$$\mathbb{H}(\mathbb{Z}) = \{n_1 + n_2 i + n_3 j + n_4 k : \underline{n} \in \mathbb{Z}^4\} \tag{27}$$

together with the points with odd half-integer coordinates,

$$\mathrm{D4} = \mathbb{H}(\mathbb{Z}) \cup \left(\mathbb{H}(\mathbb{Z}) + \frac{1}{2}(1 + i + j + k)\right). \tag{28}$$

This is a lattice tiling, which is regular of degree 24 as a graph. The 24 neighbors of 0 are the units of the corresponding quaternion algebra,

$$U_4 = \{\pm 1, \pm i, \pm j, \pm k\} \cup \left\{\frac{1}{2}(\epsilon_1 + \epsilon_2 i + \epsilon_3 j + \epsilon_4 k) : \underline{\epsilon} \in \{\pm 1\}^4\right\}. \tag{29}$$

A basis for the lattice is given by $v_1 = 1$, $v_2 = i$, $v_3 = j$, $v_4 = \frac{1}{2}(1 + i + j + k)$. In these coordinates, the neighbors of 0 are

$$\begin{aligned}&\{\pm v_1, \pm v_2, \pm v_3, \pm(2v_4 - v_1 - v_2 - v_3), \pm v_4, \pm(-v_1 + v_4), \pm(-v_2 + v_4),\\ &\pm (-v_3 + v_4), \pm(-v_1 - v_2 + v_4), \pm(-v_1 - v_3 + v_4),\\ &\pm (-v_2 - v_3 + v_4), \pm(-v_1 - v_2 - v_3 + v_4)\}.\end{aligned}$$

Let μ be uniform on the neighbors of 0. This measure has Fourier transform

$$\begin{aligned}\hat{\mu}(x_1, x_2, x_3, x_4) = \frac{1}{12}(&c(x_1) + c(x_2) + c(x_3) + c(2x_4 - x_1 - x_2 - x_3)\\ &+ c(x_4) + c(-x_1 + x_4) + c(-x_2 + x_4) + c(-x_3 + x_4)\\ &+ c(-x_1 - x_2 + x_4) + c(-x_1 - x_3 + x_4) + c(-x_2 - x_3 + x_4)\\ &+ c(-x_1 - x_2 - x_3 + x_4)).\end{aligned}$$

The Green's function is given by

$$\begin{aligned}&g_0(n_1v_1 + n_2v_2 + n_3v_3 + n_4v_4)\\ &= \frac{1}{24}\int_{\mathbb{R}^4/\mathbb{Z}^4} \frac{e(n_1x_1 + n_2x_2 + n_3x_3 + n_4x_4)}{1 - \hat{\mu}(x_1, x_2, x_3, x_4)} dx_1dx_2dx_3dx_4.\end{aligned}$$

3.5. $\mathbb{Z}^d$ **lattice.** For $d \geqslant 3$ the lattice $\mathbb{Z}^d$ has Green's function

$$g_0(\underline{n}) = \frac{1}{2d}\int_{\mathbb{R}^d/\mathbb{Z}^d} \frac{e(\underline{n}\cdot\underline{x})}{1 - \frac{1}{d}\left(c(x_1) + \cdots + c(x_d)\right)} d\underline{x}. \tag{30}$$

4. Optimization problem and computer search

In this section the spectral parameters are determined by a computer search for several tilings. Recall that

$$\gamma = \inf\left\{\sum_{x\in\mathscr{T}} 1 - c(\xi_x) : \Delta\xi \in C^1(\mathscr{T}), \xi \not\equiv 0 \bmod 1\right\}$$

and

$$\gamma_i = \inf_{\substack{S\subset\{1,2,\ldots,d\}\\ |S|=i}} \inf_{\substack{\xi\in\mathscr{H}^2_S(\mathscr{T})\\ \xi\not\equiv 0 \bmod 1}} \sum_{x\in\mathscr{T}/\mathfrak{S}_S} 1 - c(\xi_x).$$

The following arguments index harmonic modulo 1 function ξ with its prevector $\nu = \Delta\xi$, which is simpler as the prevector is integer valued. This permits an approximate ordering on prevectors in terms of their norm and the diameter of their support. The harmonic modulo 1 function is then recovered as $\xi = g * \nu$, as the following lemma demonstrates.

Lemma 6. *Let $\xi \in \ell^2(\mathscr{T})$ be harmonic modulo 1, and let $\nu = \Delta\xi$ be its prevector. Then $\xi = g_\nu$.*

Proof. Since Δ is bounded $\ell^2 \to \ell^2$ and ν is integer valued, it has finite support. Given $x \in \Lambda$, let τ_x denote translation by x, and let $\xi^x = \xi - \tau_x\xi$. Hence $\nu^x = \Delta(\xi^x) = \nu - \tau_x\nu$ is in $C^1(\mathscr{T})$. It follows from [12] that $g_{\nu^x}(y) \to 0$ as $d(0, y) \to \infty$. Since

$$\Delta(\xi^x - g_{\nu^x}) = \nu^x - \nu^x = 0$$

and since $\xi^x - g_{\nu^x}$ vanishes at infinity, it follows from the maximum modulus principle that $\xi^x = g_{\nu^x}$. As $x \to \infty$ for each fixed y, $\xi^x(y) \to \xi(y)$. Since $\xi \in \ell^2(\mathscr{T})$, it tends to 0 at infinity, and hence g_ν tends to a constant at ∞. In fact, this constant is 0, since modulo a function in $C^1(\mathscr{T})$, ν is a point mass at 0, and the convolution of g with a C^1-function tends to 0, while the convolution with a point mass either grows logarithmically in dimension 2 or tends to 0 in higher dimension. The argument may now be repeated with ξ and ν replacing ξ^x and ν^x to conclude that $\xi = g_\nu$. □

The next lemma controls cosine sums of ξ in terms of the ℓ^2-norm.

Lemma 7. *Let S be a finite or countable set, and let $\xi \in \ell^2(S)$, $\|\xi\|_\infty \leqslant \frac{1}{2}$. Define*

$$f_S(\xi) = \sum_{x\in S} 1 - c(\xi_x). \tag{31}$$

Let $\alpha > 0$, and assume $\|\xi\|_2^2 \geqslant \alpha$. Then

$$2\pi^2\alpha\left(1 - \frac{\pi^2}{3}\alpha\right) \leqslant f_S(\xi) \leqslant 2\pi^2\|\xi\|_2^2. \tag{32}$$

Proof. The Taylor series approximation for $c(x)$ on $|x| \leqslant \frac{1}{2}$,

$$c(x) = 1 - 2\pi^2x^2 + \frac{2\pi^4}{3}x^4 - \cdots,$$

is an alternating series with decreasing increments after the term $2\pi^2x^2$. Thus $f_S(\xi) \leqslant 2\pi^2\|\xi\|_2^2$. Let $0 < \lambda \leqslant 1$, and let $\xi' = \lambda\xi$ satisfy $\|\xi'\|_2^2 = \alpha$. Then $f_S(\xi') \leqslant f_S(\xi)$. Furthermore, using $\|\xi'\|_4^4 \leqslant \|\xi'\|_2^4 = \alpha^2$,

$$f_S(\xi') \geqslant 2\pi^2\|\xi'\|_2^2 - \frac{2}{3}\pi^4\|\xi'\|_4^4 \geqslant 2\pi^2\alpha - \frac{2}{3}\pi^4\alpha^2.$$

□

The following lemma is used to estimate the functionals $f(\xi)$.

Lemma 8. *Let $R \subset \mathscr{T}$, and let $\xi : \mathscr{T} \to \left(-\frac{1}{2}, \frac{1}{2}\right]$. Let*

$$\|\xi\|_{2,R^c}^2 = \sum_{x\in\mathscr{T}\setminus R} \xi_x^2. \tag{33}$$

There is a number ϑ, $|\vartheta| \leqslant 1$, such that

$$f(\xi) = \sum_{x\in R}(1 - c(\xi_x)) + 2\pi^2\|\xi\|_{2,R^c}^2 - \frac{\pi^4}{3}\|\xi\|_{2,R^c}^4 + \vartheta\frac{\pi^4}{3}\|\xi\|_{2,R^c}^4. \tag{34}$$

Proof. By Taylor approximation, for $x \in R^c$,

$$2\pi^2\xi_x^2 - \frac{2}{3}\pi^4\xi_x^4 \leqslant 1 - c(\xi_x) \leqslant 2\pi^2\xi_x^2.$$

Thus,

$$\begin{aligned}\sum_{x\in R}(1 - c(\xi_x)) + 2\pi^2\|\xi_x\|_{2,R^c}^2 - \frac{2}{3}\pi^4\|\xi\|_{2,R^c}^4 \\ \leqslant f(\xi) \leqslant \sum_{x\in R}(1 - c(\xi_x)) + 2\pi^2\|\xi\|_{2,R^c}^2,\end{aligned}$$

from which the claim follows. □

In practice, Lemma 8 is applied by calculating ξ_x on R from the Fourier integral representations in Section 3 in a neighborhood of 0, and calculating $\|\xi\|_2^2$ by Parseval.

The following two optimization programs are used to obtain a lower bound for $f(\xi)$. Let $\xi = g * \nu$, $\|\xi\|_\infty \leqslant \frac{1}{2}$. Given a set $S \subset \mathscr{T}$, a lower bound for $f(\xi)$ is obtained as the solution of the optimization program $Q(S,\nu)$:

$$\begin{aligned} &Q(S,\nu): \\ &\text{minimize:} && \sum_{d(w,S)\leqslant 1} 1 - c(x_w), \\ &\text{subject to:} && \forall u \in S,\ (\deg u)x_u - \sum_{d(w,u)=1} x_w = \nu_u \\ &&& -\frac{1}{2} \leqslant x_w \leqslant \frac{1}{2}. \end{aligned}$$

A lower bound for $Q(S,\nu)$ is the relaxed optimization program with positive constraints $P(S,\nu)$:

$$\begin{aligned} &P(S,\nu): \\ &\text{minimize:} && \sum_{d(w,S)\leqslant 1} 1 - c(x_w), \\ &\text{subject to:} && \forall u \in S,\ (\deg u)x_u + \sum_{d(w,u)=1} x_w \geqslant |\nu_u| \\ &&& -\frac{1}{2} \leqslant x_w \leqslant \frac{1}{2}. \end{aligned}$$

Note that the objective function is convex and with nondegenerate Hessian in the interior with the stronger condition $|x_w| \leqslant \frac{1}{4}$, and hence has a unique local minimum there. In order to estimate $Q(S,\nu)$ and $P(S,\nu)$ numerically, the range $\frac{1}{4} \leqslant |x_w| \leqslant \frac{1}{2}$ was split into several equal size intervals and the objective function was approximated piecewise linearly on these, obtaining a lower bound for the minimum. The minima were compared with the variables constrained to lie in each interval. Denote $P_j(S,\nu)$ and $Q_j(S,\nu)$ the programs in which both $\left[-\frac{1}{2}, -\frac{1}{4}\right]$ and $\left[\frac{1}{4}, \frac{1}{2}\right]$ are split into j equal size intervals, and the objective function interpolating linearly between the values of $c(x)$ on the endpoints. Note that the minimum of P_j and Q_j on each product of intervals is determined as a unique interior minimum or boundary value. In the examples considered in dimensions 3 and higher, $\|\xi\|_2^2$ was optimized rather than $f(\xi)$, and it was demonstrated that the extremal function is the same. Programs $Q'(S,\nu)$ and $P'(S,\nu)$ have the same constraints, but have objective function $\sum_{d(w,S)\leqslant 1} x_w^2$. Note that this objective function is convex.

The optimization programs P, P_j, P', Q, Q_j, Q' satisfy the following monotonicity properties.

Lemma 9. *The programs P, P_j, P', Q, Q_j, Q' are monotone increasing in the set S, in the sense that if $S \subset T$, then $P(S,\nu) \leqslant P(T,\nu)$, and similarly for the other programs. The programs P, P_j, P' are monotone increasing in the prevector $|\nu|$.*

Proof. Either increasing the size of the constraint set or increasing $|\nu|$ makes the solution more constrained, and thus increases the minimum. □

The programs also satisfy the following additivity property.

Lemma 10. *Let $B(S) = \{u : d(u, S) \leqslant 1\}$ be the distance 1 enlargement of S. When $S_1, S_2, \ldots, S_k$ are some sets in $\mathscr{T}$ whose distance 1 enlargements are pairwise disjoint, then $\sum_{i=1}^{k} Q(S_i, \nu) \leqslant f(\xi)$ and $\sum_{i=1}^{k} Q'(S_i, \nu) \leqslant \|\xi\|_2^2$.*

Proof. Since the sets of variables are disjoint, the sum of the optimization programs can be considered to be a single optimization program, which is then satisfied by ξ. The corresponding values for ξ are thus an upper bound on the optimum. □

Since the remaining programs P, P', P_j, Q_j are relaxations of Q and Q', the additivity property in Lemma 10 holds for these as well.

A basic estimate for the value of Q' is as follows.

Lemma 11. *Let $G = (V, E)$ be a graph, and let $v \in V$ of degree at least 2, with a single edge to each of its neighbors and no self-loops. Let $|\nu_v| = 1$. The optimization problem $P'(\{v\}, 1) = Q'(\{v\}, \nu)$ has value $\frac{1}{\deg(v)(\deg(v)+1)}$.*

Proof. When considering Q', assume without loss of generality that $\nu_v = 1$. The constraint is $(\deg v)x_v - \sum_{(v,w)\in E} x_w = 1$ and the objective function is $x_v^2 + \sum_{(v,w)\in E} x_w^2$. Evidently x_w for $(v, w) \in E$ may be assumed to be nonpositive, which proves the equality of the two programs. Since the claimed value is less than $\frac{1}{4}$, we may assume that all $|x_v| < \frac{1}{2}$ at the optimum, and thus that the optimum is achieved at an interior point. By Lagrange multipliers, there is a scalar λ such that $x_v = \lambda \deg v$ and $x_w = -\lambda$ for all $(v, w) \in E$. Thus $\lambda = \frac{1}{\deg(v)(\deg(v)+1)}$. The claim follows, since

$$\sum_{d(v,w)\leqslant 1} x_w^2 = \lambda^2 \deg(v)(\deg(v) + 1). \tag{35}$$

□

In particular, combining this lemma with Lemma 10 above proves that the extremal prevector has a bounded ℓ^1-norm.

The strategy of the arguments is now described as follows. Say two points x_i, x_t in the support of ν are 2-path connected, or just connected for short, if there is a sequence of points $x_i = x_0, x_1, \ldots, x_n = x_t$ in the support of ν such that the graph distance between x_i and x_{i+1} is at most 2. By Lemma 10, the value of the optimization programs applied with S_i separated connected components of $\operatorname{supp} \nu$ is additive. Since the value of each optimization program is translation invariant and, for a fixed ν, monotone in S, all connected components with P or Q (resp., P', Q', P_j, Q_j) value at most a fixed constant can be enumerated by starting from a base configuration and adding connected points to the set S one at a time.

The configuration ν must be in C^ρ for $\xi \in \ell^2(\mathscr{T})$, where

$$\rho = \begin{cases} 2 & d = 2, \\ 1 & d = 3, 4, \\ 0 & d \geqslant 5. \end{cases}$$

Having enumerated all feasible connected components, the search is completed by considering all methods of gluing together several connected components which produce $\nu \in C^\rho$.

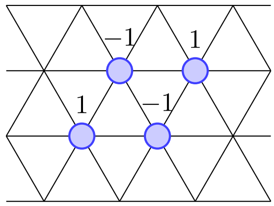

FIGURE 4. The configuration indicated is a choice of prevector ν which generates the extremal ξ for the triangular lattice.

4.1. **Issues of precision.** The techniques used in this section consist in the following: minimization of a convex function in a convex bounded region, which can be certified by the calculation of the derivative of the objective function at the optimum found, and the integration of a function with bounded derivatives over a bounded domain. Although the integrals involving the characteristic function of a Green's function may have a singularity at 0, this may be removed in each case by switching to spherical coordinates of the correct dimension near the point of singularity. Thus the numerical results are verifiable to within the claimed precision. The generating code written in SciPy is available from the public repository `https://github.com/rdhough/spectral_gap`.

4.2. **Proof of Theorems 1 and 2.**

4.2.1. *Triangular lattice case (see Figure 4).* Let the triangular lattice be generated by $v_1 = (1,0)$ and $v_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$. Let $\xi^* = g * \nu^*$ with $\nu^* = \delta_0 - \delta_{v_1} - \delta_{v_2} + \delta_{v_1+v_2}$. The value

$$f(\xi^*) = 1.69416(5) \tag{36}$$

was estimated by Lemma 8 with

$$R = \{n_1 v_1 + n_2 v_2 : \max(|n_1|, |n_2|) \leqslant 10\}. \tag{37}$$

It is shown that $\gamma_{\mathrm{tri}} = f(\xi^*)$ by computer search. The documentation and source code for this search are available from the public repository `https://github.com/rdhough/spectral_gap`.

4.2.2. *Honeycomb tiling case (see Figure 5).* Let $v_1 = (1,0)$, let $v_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$, and let $v = \frac{1}{3}(v_1 + v_2)$. Thus the points in the honeycomb lattice have the form $n_1 v_1 + n_2 v_2 + n_3 v$ with $n_3 \in \{0,1\}$ and $n_1, n_2 \in \mathbb{Z}$. The optimal configuration is given by $\xi^* = g * \nu^*$:

$$\nu^* = \delta_0 - \delta_v + \delta_{v_2} - \delta_{-v_1+v} + \delta_{v_2-v_1} - \delta_{v_2-v_1+v}. \tag{38}$$

The value $f(\xi^*) = 5.977657(8)$ was obtained as in Lemma 8 with

$$R = \{n_1 v_1 + n_2 v_2 + n_3 v : |n_1|, |n_2| \leqslant 10, n_3 \in \{0,1\}\}. \tag{39}$$

The documentation of this computer search, and its source code, are available from the public repository `https://github.com/rdhough/spectral_gap`.

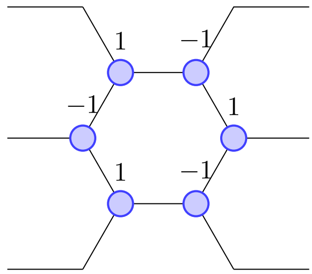

FIGURE 5. The configuration indicated is a choice of prevector ν which generates the extremal ξ for the honeycomb tiling.

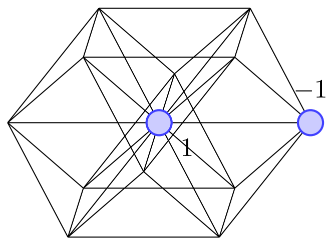

FIGURE 6. The configuration indicated is a choice of prevector ν which generates the extremal ξ for the face centered cubic lattice.

4.2.3. *Face centered cubic lattice case (see Figure 6).* The optimum is shown to be achieved by $\nu^* = \delta_0 - \delta_{v_1}$, $\xi^* = g * \nu^*$ with $\|\xi^*\|_2^2 = 0.01867(5)$. The value $\gamma_{\text{fcc}} = f(\xi^*) = 0.3623(9)$ was calculated by applying Lemma 8 with

$$R = \{n_1 v_1 + n_2 v_2 + n_3 v_3 : |n_1|, |n_2|, |n_3| \leqslant 5\}. \tag{40}$$

In order to show that ν^* is the optimizer, it is more convenient to work with $\|\xi\|_2^2$ than $f(\xi)$. By Lemma 7, if $\|\xi\|_2^2 \geqslant \alpha$ with

$$2\pi^2\alpha\left(1 - \frac{\pi^2}{3}\alpha\right) > \gamma_{\text{fcc}}, \qquad \alpha = 0.01963, \tag{41}$$

then $f(\xi) > \gamma_{\text{fcc}}$.

Let ξ be harmonic modulo 1, $\|\xi\|_\infty \leqslant \frac{1}{2}$. Let $\Delta\xi = \nu$.

Lemma 12. *If $\|\nu\|_\infty \geqslant 2$, then $\|\xi\|_2^2 \geqslant \frac{4}{12\cdot 13} > 0.025 > \alpha$.*

Proof. By Lemma 11, since $\deg(0) = 12$, $P'(\{0\}, 1) = \frac{1}{12\cdot 13}$. Within the interior of the domain, the objective function scales quadratically, and hence $P'(\{0\}, 2) = \frac{4}{12\cdot 13}$. Applying this, translated to node x where $|\nu_x| \geqslant 2$, implies the claim. □

Since the Green's function on a three-dimensional lattice is not in ℓ^2, it follows that the optimal ν is in $C^1(\mathscr{T})$, and hence has the same number of nodes with values 1 and −1.

Lemma 13. *Suppose $|\operatorname{supp}\nu| \geqslant 4$, and let z_1, z_2, z_3, z_4 be four points in the support, two each with value $1, -1$. The optimization problem $Q'(\{z_1, z_2, z_3, z_4\}, \nu)$ has value at least $\frac{2}{99} > \alpha$.*

Proof. Let the linear constraints be written as $\ell_i \cdot x = \nu_{z_i}$. Thus ℓ_i has value 12 at z_i and value -1 at each of the 12 neighbors of z_i. Recall that the optimization problem minimizes $\|x\|_2^2$ subject to the constraints. The optimum can be assumed not to be achieved on the boundary, since if some $|x_j| = \frac{1}{2}$, then $\|x\|_2^2 \geqslant \frac{1}{4}$, which exceeds the claimed bound. By Lagrange multipliers, at the optimum, for some scalars $\lambda_1, \lambda_2, \lambda_3, \lambda_4$, $x = \lambda_1\ell_1 + \lambda_2\ell_2 + \lambda_3\ell_3 + \lambda_4\ell_4$. Note that $\|\ell_i\|_2^2 = 12 \cdot 13 = 156$. Also, for $i \neq j$, $-20 \leqslant \ell_i \cdot \ell_j \leqslant 2$. The lower bound here is achieved when z_i and z_j are adjacent, in which case they have four common neighbors. The upper bound is achieved when they differ by a rotation of $v_1 + v_2$, in which case they have two common neighbors.

The constraints may be written as

$$\ell_i^t(\lambda_1\ell_1 + \lambda_2\ell_2 + \lambda_3\ell_3 + \lambda_4\ell_4) = \nu_{z_i} \tag{42}$$

or

$$156(I + A)\begin{pmatrix}\lambda_1\\ \lambda_2\\ \lambda_3\\ \lambda_4\end{pmatrix} = \begin{pmatrix}\nu_{z_1}\\ \nu_{z_2}\\ \nu_{z_3}\\ \nu_{z_4}\end{pmatrix}, \tag{43}$$

where A has zeros on the diagonal and has row sums contained in the interval $[-\frac{60}{156}, \frac{6}{156}]$. Let $\lambda_i' = 156\lambda_i$ and rewrite this as

$$A\begin{pmatrix}\lambda_1'\\ \lambda_2'\\ \lambda_3'\\ \lambda_4'\end{pmatrix} = \begin{pmatrix}\nu_{z_1} - \lambda_1'\\ \nu_{z_2} - \lambda_2'\\ \nu_{z_3} - \lambda_3'\\ \nu_{z_4} - \lambda_4'\end{pmatrix}. \tag{44}$$

Thus $\max(|\nu_{z_i} - \lambda_i'|) \leqslant \frac{60}{156}\max(|\lambda_i'|)$. Since $|\nu_{z_i}| = 1$, it follows that $\max(|\lambda_i'|) \leqslant 2$, and, hence, $\max(|\nu_{z_i} - \lambda_i'|) \leqslant \frac{120}{156} < 1$. Thus λ_i and ν_{z_i} have the same sign.

Write

$$(\nu_{z_1}\ell_1 + \nu_{z_2}\ell_2 + \nu_{z_3}\ell_3 + \nu_{z_4}\ell_4)^t(\lambda_1\ell_1 + \lambda_2\ell_2 + \lambda_3\ell_3 + \lambda_4\ell_4) = 4,$$

and, by expanding the inner product on the left, express this as

$$\begin{aligned} &a_1\nu_{z_1}\lambda_1 + a_2\nu_{z_2}\lambda_2 + a_3\nu_{z_3}\lambda_3 + a_4\nu_{z_4}\lambda_4 \\ &\quad = a_1|\lambda_1| + a_2|\lambda_2| + a_3|\lambda_3| + a_4|\lambda_4| = 4, \end{aligned}$$

where

$$a_i = \|\ell_i\|_2^2 + \sum_{j \neq i} \nu_{z_i}\nu_{z_j}\ell_i \cdot \ell_j.$$

There is one j for which $\nu_{z_i} = \nu_{z_j}$ and two of the opposite sign. Since $-20 \leqslant \ell_i \cdot \ell_j \leqslant 2$,

$$-24 \leqslant \sum_{j \neq i} \nu_{z_i}\nu_{z_j}\ell_i \cdot \ell_j \leqslant 42.$$

By the above considerations, $156 - 24 = 132 \leqslant a_i \leqslant 156 + 42 = 198$. Since

$$\begin{aligned} \|x\|_2^2 &= \lambda_1\nu_{z_1} + \lambda_2\nu_{z_2} + \lambda_3\nu_{z_3} + \lambda_4\nu_{z_4} \\ &= |\lambda_1| + |\lambda_2| + |\lambda_3| + |\lambda_4| \end{aligned}$$

it follows that $\|x\|_2^2 \geqslant \frac{4}{198} = 0.\overline{02} > \alpha$. □

It follows that the optimum has $|\operatorname{supp}\nu| = 2$. The following lemma reduces the search to a finite search.

Lemma 14. *Let $|\nu_0| = 1$, and let $\nu_w = 0$ for w such that $1 \leqslant d(w,0) \leqslant 2$. Let $S = \{w : d(w,0) \leqslant 2\}$. Then $Q'(S,\nu) \geqslant 0.0125$.*

Proof. This was verified in SciPy. □

It follows that there may not be two points in the support of ν at graph distance greater than 6, or else the optimization problem could be applied at each point, and the 2-norm would be too large. This reduces the search to checking all configurations with two points in the support at graph distance at most 6. The choice with adjacent points is the minimizer.

4.2.4. D4 *tiling case.* The following optimization problems are used in the determination of the spectral parameters. In D4, up to multiplication by a unit and reflection in the coordinate hyperplanes, there is one element each of norm 1, 2, 3, and 4 in D4. Representatives are 1, $1+i$, $1+i+j$, and 2.

Lemma 15. *Consider the following optimization problems:*

(i) *Let $\nu_0 = 1$. Then*

$$P'(\{0\},1) = \frac{1}{600} = 0.001\overline{6}. \tag{45}$$

(ii) *Let $S = \{w : d(w,0) \leqslant 1\}$. Let $\nu_0 = 1$, and let $\nu_w = 0$ for w such that $d(w,0) = 1$. Then*

$$Q'(S,\nu) \geqslant 0.00206. \tag{46}$$

(iii) *Let $\nu_0 = 1$, and let $\nu_w = 0$ for $1 \leqslant d(w,0) \leqslant 2$. Then*

$$Q'(S,\nu) \geqslant 0.00233. \tag{47}$$

(iv) *For $u \in \{1, 1+i, 1+i+j, 2\}$ let $\nu_0 = 1$, $\nu_u = \pm 1$. A lower bound for the program $Q'(\{0,u\},\nu)$ in each case is given in the following table:*

u	$+1$	-1
1	0.00357	0.00312
$1+i$	0.00330	0.00336
$1+i+j$	0.00332	0.00334
2	0.00332	0.00333

Proof. The first value is the same as from Lemma 11. The remaining values were determined in SciPy. □

Note that the first estimate of the lemma implies that $P'(\{0\},2) \geqslant \frac{1}{150}$, since the objective function is quadratic. This reduces to prevectors with $\|\nu\|_\infty \leqslant 1$ in the calculations that follow.

Lemma 16. *If ξ is harmonic modulo 1 on D4 and $\nu = \Delta\xi$ has $|\operatorname{supp}\nu| \geqslant 3$, then $\|\xi\|_2^2 \geqslant \frac{3}{742} > 0.004043$.*

Proof. Let z_1, z_2, z_3 be points in the support of ν. Then $\|\xi\|_2^2$ is bounded below by the value of the relaxed optimization program $P'(\{z_1,z_2,z_3\},1)$. By applying Lagrange multipliers, the variable x may be expressed as $\lambda_1 v_1 + \lambda_2 v_2 + \lambda_3 v_3$, where v_1, v_2, v_3 are the gradients of the constraint linear forms. The linear constraints become $v_i^t(\lambda_1 v_1 + \lambda_2 v_2 + \lambda_3 v_3) = 1$ and

$$\|x\|_2^2 = (\lambda_1 v_1 + \lambda_2 v_2 + \lambda_3 v_3)^t(\lambda_1 v_1 + \lambda_2 v_2 + \lambda_3 v_3) = \lambda_1 + \lambda_2 + \lambda_3. \tag{48}$$

Since each v_i has one entry 24 and 24 entries 1, $\|v_i\|_2^2 = 600$, and for $i \neq j$, $v_i^t v_j \leqslant 24 + 24 + 23 = 71$. Write the constraints as

$$600(I + A)\begin{pmatrix}\lambda_1\\ \lambda_2\\ \lambda_3\end{pmatrix} = \begin{pmatrix}1\\1\\1\end{pmatrix} \tag{49}$$

with A having 0's on the diagonal and row sums bounded in size by $\frac{142}{600}$. Let $\lambda_i' = 600\lambda_i$, so that

$$A\begin{pmatrix}\lambda_1'\\ \lambda_2'\\ \lambda_3'\end{pmatrix} = \begin{pmatrix}1-\lambda_1'\\ 1-\lambda_2'\\ 1-\lambda_3'\end{pmatrix}, \tag{50}$$

so that $\max(|1 - \lambda_i'|) \leqslant \frac{142}{600}\max(|\lambda_i'|)$. This implies that $\max(|\lambda_i'|) \leqslant 2$ and thus $\max(|1-\lambda_i'|) \leqslant \frac{284}{600}$, so that each $\lambda_i > 0$. Thus, summing constraints, $\lambda_1+\lambda_2+\lambda_3 \geqslant \frac{3}{742}$. □

The proof of Theorem 1 in the case of D4 is as follows.

Case ($\gamma_{\mathrm{D4},0}$). The extremal example is given by $\xi^* = g * \nu^*$ with $\nu^* = \delta_0 - \delta_1$.

The 2-norm of ξ^* was calculated by Parseval,

$$\begin{aligned}\|\xi^*\|_2^2 &= \int_{(\mathbb{R}/\mathbb{Z})^4} \frac{2(1 - c(y_1))}{g(y_1, y_2, y_3, y_4)^2} dy_1 dy_2 dy_3 dy_4,\\ g(y_1, y_2, y_3, y_4) &= 24 - 2(c(y_1) + c(y_2) + c(y_3) + c(2y_4 - y_1 - y_2 - y_3)\\ &\quad + c(y_4) + c(y_4 - y_1 - y_2 - y_3) + c(y_4 - y_1) + c(y_4 - y_2)\\ &\quad + c(y_4 - y_3) + c(y_4 - y_1 - y_2) + c(y_4 - y_1 - y_3)\\ &\quad + c(y_4 - y_2 - y_3)).\end{aligned}$$

This was calculated in SciPy, $\|\xi^*\|_2^2 = 0.0038397(3)$. By symmetry, $\|\xi^*\|_\infty^2 \leqslant \frac{1}{2}\|\xi^*\|_2^2$, and hence $\|\xi^*\|_4^4 \leqslant \frac{1}{2}\|\xi^*\|_2^4$. It follows that, for some $|\vartheta| < 1$, whose value may vary from line to line,

$$\begin{aligned}\gamma_{\mathrm{D4},0} &= 2\pi^2\|\xi^*\|_2^2 - \frac{\pi^4}{3}\|\xi^*\|_4^4 + \vartheta\frac{\pi^4}{3}\|\xi^*\|_4^4\\ &= 2\pi^2\|\xi^*\|_2^2 - \frac{\pi^4}{6}\|\xi^*\|_2^4 + \vartheta\frac{\pi^4}{6}\|\xi^*\|_2^4\\ &= 0.075554 + \vartheta 0.00024.\end{aligned}$$

Thus,

$$\Gamma_{\mathrm{D4},0} = \frac{4}{\gamma_0} = 52.9428 + \vartheta 0.17.$$

To verify that ξ^* is extremal, suppose that ξ is harmonic modulo 1, $\|\xi\|_\infty \leqslant \frac{1}{2}$, and $\Delta\xi = \nu$ is another candidate. Since the Green's function is not in ℓ^2 in dimension 4, it follows that $\nu \in C^1(\mathscr{T})$. By Lemma 7, to conclude that ξ is not extremal, it suffices to conclude that $\|\xi\|_2^2 \geqslant \alpha$ with

$$2\pi^2\alpha\left(1 - \frac{\pi^2}{3}\alpha\right) \geqslant 0.075794, \qquad \alpha > 0.0039. \tag{51}$$

Note that $\|\nu\|_\infty = 1$, since the first optimization program in Lemma 15 can be applied where $|\nu_x| \geqslant 2$ and gives a value for the 2-norm which is too large. Also, there are not 3 points in $\operatorname{supp}\nu$ by Lemma 16. If the two points in the support of ν have distance at least 5, then the second optimization problem of Lemma 15 may be applied at each point, which makes the 2-norm too large. Hence the two points in the support have graph distance at most 4. One point may be taken to be 0. The second point needs to be considered only up to multiplication by the 24 quaternion units and by reflection in the coordinate hyperplanes. The candidates for the second point were checked exhaustively; the minimizer is ν_0 and all other points had a 2-norm too large.

Case ($\gamma_{\mathrm{D4},1}$). By symmetry assume that the reflecting hyperplane is $\mathscr{P}_1 = \{x \in \mathbb{R}^4 : x_1 + x_2 = 0\}$. It is verified that the optimal prevector is $\nu^* = \delta_{(1,0,0,0)}$, with reflection symmetry, so that $\nu^*(0,-1,0,0) = -1$, and let $\xi^* = g * \nu^*$. The 2-norm may be taken on the quotient by summing ξ_x^2 over points x on one side of the hyperplane, including the hyperplane where ξ vanishes, hence say

$$\|\xi\|_{2,\{1\}}^2 = \sum_{x : x_1 + x_2 \geqslant 0} \xi_x^2. \tag{52}$$

By Parseval,

$$\|\xi^*\|_{2,\{1\}}^2 = \frac{1}{2}\int_{(\mathbb{R}/\mathbb{Z})^4} \frac{|e(y_1) - e(-y_2)|^2}{g(y_1,y_2,y_3,y_4)^2} dy_1 dy_2 dy_3 dy_4 = 0.0022421(8). \tag{53}$$

In this case

$$\begin{aligned}\gamma_{\mathrm{D4},1} &= 2\pi^2 \|\xi^*\|_{2,\{1\}}^2 - \frac{\pi^4}{3}\|\xi^*\|_{2,\{1\}}^4 + \vartheta\frac{\pi^4}{3}\|\xi^*\|_{2,\{1\}}^4 \\ &= 0.0440957 + \vartheta 0.00017.\end{aligned}$$

Thus,

$$\Gamma_{\mathrm{D4},1} = \frac{3}{\gamma_1} = 68.03486 + \vartheta 0.27.$$

To check that ξ^* is the optimizer, let ξ be harmonic modulo 1, let $\|\xi\|_\infty \leqslant \frac{1}{2}$, with reflection antisymmetry in $\mathscr{P}_1$, and let $\Delta\xi = \nu$. It suffices to prove by Lemma 7 that $\|\xi\|_{2,\{1\}}^2 \geqslant \alpha$ with

$$2\pi^2\alpha\left(1 - \frac{\pi^2}{3}\alpha\right) \geqslant 0.04427, \qquad \alpha > 0.00226. \tag{54}$$

If $|\operatorname{supp}\nu| \geqslant 2$ in $\{x : x_1 + x_2 > 0\}$, then if two of the points in the support have distance at least 3 apart, the first optimization problem of Lemma 15 may be applied at each point. Otherwise the last optimization problem may be applied. In either case, the 2-norm is too large. Thus there is a single point in the support, say (x_1, x_2, x_3, x_4) of value 1. The reflection point is $(-x_2, -x_1, x_3, x_4)$. The 2-norm is, by Parseval,

$$\int_{(\mathbb{R}/\mathbb{Z})^4} \frac{|e(x_1y_1 + x_2y_2) - e(-x_2y_1 - x_1y_2)|^2}{g(y_1,y_2,y_3,y_4)^2} dy_1 dy_2 dy_3 dy_4. \tag{55}$$

If x has graph distance 3 or more from the boundary hyperplane $\mathscr{P}_1$, then the third optimization program of Lemma 15 may be applied to show that the 2-norm is too large. It now follows by checking case by case that the minimizer is $z = x_1 + x_2 = 1$, which is ν^*.

Case ($\gamma_{\mathrm{D}4,2}$). By symmetry assume that the reflecting hyperplanes are $\mathscr{P}_1 = \{x \in \mathbb{R}^4 : x_1 + x_2 = 0\}$ and $\mathscr{P}_2 = \{x \in \mathbb{R}^4 : x_1 - x_2 = 0\}$. The optimizing prevector is $\nu^* = \delta_{(1,0,0,0)}$ and $\xi^* = g * \nu^*$. By reflection antisymmetry,

$$\nu^*(0,-1,0,0) = -1, \qquad \nu^*(-1,0,0,0) = 1, \qquad \nu^*(0,1,0,0) = -1. \tag{56}$$

The 2-norm is $\|\xi^*\|^2_{2,\{1,2\}} = 0.0019800(3)$. Calculating as in the case of $\gamma_{\mathrm{D}4,1}$,

$$\begin{aligned}\gamma_{\mathrm{D}4,2} &= 2\pi^2\|\xi^*\|^2_{2,\{1,2\}} - \frac{\pi^4}{3}\|\xi^*\|^4_{2,\{1,2\}} + \vartheta\frac{\pi^4}{3}\|\xi^*\|^4_{2,\{1,2\}} \\ &= 0.0389569 + \vartheta 0.00013.\end{aligned}$$

Thus,

$$\Gamma_{\mathrm{D}4,2} = \frac{2}{\gamma_{\mathrm{D}4,2}} = 51.3393 + \vartheta 0.17.$$

To verify that ξ^* is extremal, let ξ be harmonic modulo 1 with reflection antisymmetry in $\mathscr{P}_1$ and $\mathscr{P}_2$, and let $\nu = \Delta\xi$. To rule out that ξ is extremal it suffices to check by Lemma 7 that $\|\xi\|^2_{2,\{1,2\}} \geqslant \alpha$ with

$$2\pi^2\alpha\left(1 - \frac{\pi^2}{3}\alpha\right) \geqslant 0.0391, \qquad \alpha > 0.002. \tag{57}$$

The case of two points in the support modulo reflections is ruled out as before. Suppose the point in the support is (x_1,x_2,x_3,x_4). This point may have not have distance at least 2 from both hyperplanes, or else the second optimization problem of Lemma 15 may be applied to show that the 2-norm is too large. Hence, $\min(|x_1 + x_2|, |x_1 - x_2|) = 1$, say, by symmetry, $x_1 + x_2 = 1$, and x differs by $(1,1,0,0)$ from its reflection in $\mathscr{P}_1$. If x has graph distance 3 or more from $\mathscr{P}_2$, then the optimization program which enforces $\Delta\xi(0,0,0,0) = 1$, $\Delta\xi(1,1,0,0) = -1$ and $\Delta\xi(v) = 0$ if $d(v, \{(0,0,0,0),(1,1,0,0)\}) \leqslant 2$ can be applied, which has minimum 2-norm $0.0041780(9)$. This is a lower bound for twice the 2-norm of ξ modulo reflections, and is too large. Hence x has graph distance at most 2 from $\mathscr{P}_2$, so $x_1 - x_2$ is either 1 or 2. The case 1 is the minimizer.

Case ($\gamma_{\mathrm{D}4,3}$). By symmetry assume the reflecting hyperplanes are $\mathscr{P}_1, \mathscr{P}_2, \mathscr{P}_3$, with

$$\mathscr{P}_3 = \{x \in \mathbb{R}^4 : x_3 + x_4 = 0\}. \tag{58}$$

It is shown that the minimizer is $\nu^* = \delta_{(1,0,1,0)}$ with $\xi^* = g * \nu^*$, $\|\xi^*\|^2_{2,\{1,2,3\}} = 0.0018737(9)$. The corresponding value of α to rule out other configurations is $\alpha = 0.00189$. Arguing as for $\gamma_{\mathrm{D}4,1}$ and $\gamma_{\mathrm{D}4,2}$,

$$\gamma_{\mathrm{D}4,3} = 0.036873324 + \vartheta 0.00012.$$

Thus,

$$\Gamma_{\mathrm{D}4,3} = \frac{1}{\gamma_{\mathrm{D}4,3}} = 27.1201 + \vartheta 0.084.$$

Arguing as above, we may assume that $|\operatorname{supp}\nu^*| = 1$, and that the point $x = (x_1,x_2,x_3,x_4)$ has distance 1 to one hyperplane, say, without loss, that $x_1 + x_2 = 1$. Also, the distance to the next closest hyperplane is at most 2, so say $x_1 - x_2 = 1$ or $x_1 - x_2 = 2$. If $\operatorname{supp}\nu$ had distance 3 or more from $\mathscr{P}_3$, then after translation, the program $Q'(S,\nu)$ can be applied with S given by $\operatorname{supp}\nu$ together with its reflection in $\mathscr{P}_1$ and $\mathscr{P}_2$, and the distance 2 neighborhood of these points, the corresponding lower bound being $\frac{1}{4}$ of this value due to the reflections. Up to translation, this reduces to considering $\Delta\xi$ at

$$(0,0,0,0),(1,1,0,0),(1,-1,0,0),(2,0,0,0)$$

or

$$(0,0,0,0),(1,1,0,0),(2,-2,0,0),(3,-1,0,0)$$

and their distance 2 neighborhood. Both programs were ruled out. The three remaining possibilities are considered, and ν^* gives the optimum.

Case ($\gamma_{\mathrm{D}4,4}$). The minimizer is $\nu^* = \delta_{(1,0,1,0)}$ with $\xi^* = g * \nu^*$, $\|\xi^*\|^2_{2,\{1,2,3,4\}} = 0.0018170(7)$. The value of α to rule out other configurations in this case is $\alpha = 0.0018281$. This obtains

$$\gamma_{\mathrm{D}4,4} = 0.0357604 + \vartheta 0.00011.$$

The above considerations reduce to the case where ν is supported at a single point, with distance 1 from $\mathscr{P}_1$, and distance at most 2 from $\mathscr{P}_2$ and $\mathscr{P}_3$. Arguing similarly to the case of three hyperplanes shows that the distance to $\mathscr{P}_4$ is also at most 2, which reduces to a finite check. The best case is ν^*.

5. The spectral parameters of the $\mathbb{Z}^d$-tiling

This section evaluates the spectral factor of the $\mathbb{Z}^d$-lattice asymptotically, proving Theorem 3.

When $d \geqslant 3$, the Green's function on $\mathbb{Z}^d$ may be recovered from its Fourier transform via Fourier inversion,

$$g_0(x) = \frac{1}{2d}\int_{(\mathbb{R}/\mathbb{Z})^d} \frac{e(x\cdot y)}{1-\frac{1}{d}(c(y_1)+\cdots+c(y_d))}dy. \tag{59}$$

The following lemma is useful in studying this integral evaluation asymptotically. Let meas denote the unit Lebesgue measure on $[0,1]$.

Lemma 17. *Let $X_1, X_2, \ldots, X_d$ be i.i.d. random variables on $[-1,1]$ with distribution*

$$\mathbf{Prob}(X_1 \leqslant a) = \mathrm{meas}\,\{0 \leqslant t \leqslant 1 : c(t) \leqslant a\}. \tag{60}$$

Let $X = \frac{1}{d}(X_1 + X_2 + \cdots + X_d)$. For $0 \leqslant \delta \leqslant 1$,

$$\mathbf{Prob}(X > 1-\delta) \leqslant \min\left(e^{-\frac{d(1-\delta)^2}{2}}, \left(\frac{\pi e \delta}{4}\right)^{\frac{d}{2}}\right). \tag{61}$$

The two bounds are equal for $\delta = 0.27819(3) =: \zeta$.

Proof. Chernoff's inequality [1, p. 328, Theorem A.1.16] states that if $Y_1, \ldots, Y_n$ are independent with $\mathbf{E}[Y_i] = 0$ and $|Y_i| \leqslant 1$, with $S = Y_1 + \cdots + Y_n$, then

$$\mathbf{Prob}(S > a) < e^{-\frac{a^2}{2n}}.$$

The first claimed bound follows, since $\mathbf{E}[X_1] = 0$ and $|X_1| \leqslant 1$. For the second bound, use $1 - c(t) \geqslant 8t^2$ for $|t| \leqslant \frac{1}{2}$. Thus, estimating with the Euclidean volume of a ball of radius r in d dimensions, $\mathrm{vol}\, B_r(0) = \frac{r^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}$,

$$\mathbf{Prob}(X > 1-\delta) \leqslant \mathrm{meas}\left(\underline{t} \in \left[-\frac{1}{2}, \frac{1}{2}\right]^d : \|\underline{t}\|_2^2 \leqslant \frac{\delta d}{8}\right) \leqslant \frac{(\pi\delta d)^{\frac{d}{2}}}{8^{\frac{d}{2}}\Gamma\left(\frac{d}{2}+1\right)}. \tag{62}$$

Now use

$$\Gamma\left(\frac{d}{2}+1\right) \geqslant \left(\frac{d}{2e}\right)^{\frac{d}{2}}, \tag{63}$$

which is valid for $d \geqslant 2$. □

The following lemma estimates $\|\xi\|_2^2$ asymptotically when ν is supported on a single point. This example controls the mixing time for all d sufficiently large.

Lemma 18. *Let $d \geqslant 5$, let $0 \leqslant k \leqslant d$, and let $\nu : \mathbb{Z}^d \to \mathbb{Z}$ which has reflection antisymmetry in the first k coordinate hyperplanes $\mathscr{P}_1, \dots, \mathscr{P}_k$. Let $\mathfrak{S}_k$ be the group of reflections in $\mathscr{P}_1, \dots, \mathscr{P}_k$ and suppose that modulo $\mathfrak{S}_k$, ν is a point mass. Let $\xi = g * \nu$. Then as $d \to \infty$,*

$$\|\xi\|^2_{2,\mathbb{Z}^d/\mathfrak{S}_k} = \frac{1}{4d^2}\left(1 + \frac{3}{2d} + O_k\left(d^{-2}\right)\right). \tag{64}$$

Proof. When $d \geqslant 5$ the Green's function is in $\ell^2(\mathbb{Z}^d)$. The ℓ^2-norm is

$$\|g_0\|_2^2 = \frac{1}{4d^2}\int_{(\mathbb{R}/\mathbb{Z})^d} \frac{dy}{\left(1 - \frac{1}{d}\left(c(y_1) + \cdots + c(y_d)\right)\right)^2}. \tag{65}$$

Note that $\frac{1}{d}\left(c(y_1) + \cdots + c(y_d)\right)$ is the Fourier series of the measure μ of a simple random walk on $\mathbb{Z}^d$.

When ν has reflection symmetry in k hyperplanes and is supported at a single point a in the quotient space, the 2-norm of $g * \nu$ in the quotient space is

$$\begin{aligned}\|g * \nu\|^2_{2,\mathbb{Z}^d/\mathfrak{S}_k} &= \frac{1}{4d^2}\int_{(\mathbb{R}/\mathbb{Z})^d} \frac{\frac{1}{2^k}\left|\prod_{j=1}^k (e(a_j y_j) - e(-a_j y_j))\right|^2}{\left(1 - \frac{1}{d}\left(c(y_1) + \cdots + c(y_d)\right)\right)^2} dy \\ &= \frac{1}{4d^2}\int_{(\mathbb{R}/\mathbb{Z})^d} \frac{\prod_{j=1}^k (1 - c(2a_j y_j))}{\left(1 - \frac{1}{d}\left(c(y_1) + \cdots + c(y_d)\right)\right)^2} dy.\end{aligned}$$

By symmetry of the random walk,

$$\|g * \nu\|^2_{2,\mathbb{Z}^d/\mathfrak{S}_k} = \frac{1}{4d^2}\int_{(\mathbb{R}/\mathbb{Z})^d} \frac{\prod_{j=1}^k (1 - e(2a_j y_j))}{\left(1 - \frac{1}{d}\left(c(y_1) + \cdots + c(y_d)\right)\right)^2} dy. \tag{66}$$

Use the formula

$$\frac{1}{(1-x)^2} = 1 + 2x + 3x^2 + \cdots + nx^{n-1} + \frac{nx^n}{1-x} + \frac{x^n}{(1-x)^2} \tag{67}$$

with $x = \frac{1}{d}\left(c(y_1) + \cdots + c(y_d)\right)$.

To estimate $\|g_0\|_2^2$, write this as

$$\begin{aligned}\|g_0\|_2^2 &= \frac{1}{4d^2}\left(1 + 3\int_{(\mathbb{R}/\mathbb{Z})^d} x^2 dy + 4\int_{(\mathbb{R}/\mathbb{Z})^d} \frac{x^4}{1-x} dy + \int_{(\mathbb{R}/\mathbb{Z})^d} \frac{x^4}{(1-x)^2} dy\right) \\ &= \frac{1}{4d^2}\left(1 + \frac{3}{2d} + \int_{(\mathbb{R}/\mathbb{Z})^d} \frac{4x^4}{1-x} + \frac{x^4}{(1-x)^2} dy\right).\end{aligned}$$

To estimate the integrals, by symmetry, pair x and $-x$ so that the integrals become

$$-\int_0^1 c^4\left(\frac{8}{1-c^2}+\frac{2+2c^2}{(1-c^2)^2}\right)d\mathbf{Prob}(x \geqslant c)$$
$$=\int_0^1 \frac{d}{dc}\left(\frac{c^4(10-6c^2)}{(1-c^2)^2}\right)\mathbf{Prob}(x \geqslant c)dc$$
$$=\int_0^1 \left(\frac{40c^3-36c^5}{(1-c^2)^2}+\frac{40c^5-24c^7}{(1-c^2)^3}\right)\mathbf{Prob}(x \geqslant c)dc$$
$$\leqslant \int_0^{1-\zeta}\left(\frac{40c^3+12c^7}{(1-c^2)^3}\right)e^{-\frac{dc^2}{2}}dc \tag{68}$$
$$+\int_0^{\zeta}\left(\frac{40(1-c)^3+12(1-c)^7}{c^3(2-c)^3}\right)\left(\frac{\pi e c}{4}\right)^{\frac{d}{2}}dc. \tag{69}$$

In (68), bound $\frac{1}{1-c^2} \leqslant \frac{1}{2\zeta-\zeta^2}$, and then extend the integrals to ∞ to obtain a bound of $O(d^{-2})$. The integral (69) is exponentially small in d.

Also, for $a \neq 0$, writing

$$1+2x+3x^2+4x^3+4\frac{x^4}{1-x}+\frac{x^4}{(1-x)^2}$$

and bounding the integral of the last two terms in absolute value obtains

$$\frac{1}{4d^2}\int_{(\mathbb{R}/\mathbb{Z})^d}\frac{e(2\sum_{j=1}^k a_j y_j)}{\left(1-\frac{1}{d}\left(c(y_1)+\cdots+c(y_d)\right)\right)^2}dy$$
$$=\frac{3}{4d^2}\mu^{*2}(2a_1e_1+\cdots+2a_ke_k)+O\left(\frac{1}{4d^2}\int_{(\mathbb{R}/\mathbb{Z})^d}\frac{x^4}{(1-x)^2}dy\right)$$
$$=\frac{3}{16d^4}\mathbf{1}(\|a_1e_1+\cdots+a_ke_k\|_1=1)+O\left(\frac{1}{d^4}\right).$$

By expanding the numerator of (66), this implies that

$$\|g*\nu\|^2_{2,\mathbb{Z}^d/\mathfrak{S}_k}=\frac{1}{4d^2}\left(1+\frac{3}{2d}+O_k(d^{-2})\right). \tag{70}$$

□

The following lemma evaluates $\|\xi\|_2^2$ asymptotically when the support of ν is larger.

Lemma 19. *Let $d \geqslant 5$. Let $\nu=\delta_0-\delta_a$ for some $a \neq 0 \in \mathbb{Z}^d$, and let $\xi = g*\nu$. As $d \to \infty$,*

$$\|\xi\|_2^2=\begin{cases}\frac{1}{2d^2}\left(1+\frac{1}{2d}+O\left(d^{-2}\right)\right) & \|a\|_1=1,\\ \frac{1}{2d^2}\left(1+\frac{3}{2d}+O\left(d^{-2}\right)\right) & \|a\|_1>1.\end{cases} \tag{71}$$

Proof. As in the previous lemma, let $\hat{\mu}(y) = \frac{1}{d}(c(y_1) + \cdots + c(y_d))$. Then, by Parseval, estimating the error as above,

$$\begin{aligned}\|g * \nu\|_2^2 &= \frac{1}{4d^2} \int_{(\mathbb{R}/\mathbb{Z})^d} \frac{|\hat{\nu}(y)|^2}{(1-\hat{\mu}(y))^2} dy \\ &= \frac{1}{4d^2} \int_{(\mathbb{R}/\mathbb{Z})^d} |\hat{\nu}(y)|^2 \left(1 + 2\hat{\mu}(y) + 3\hat{\mu}(y)^2 + 4\hat{\mu}(y)^3\right) dy + O(d^{-4}).\end{aligned}$$

Let $\check{\nu}(x) = \nu(-x)$. The integral can be evaluated by using Parseval on each term,

$$\int_{(\mathbb{R}/\mathbb{Z})^d} |\hat{\nu}(y)|^2 \hat{\mu}(y)^j dy = \nu * \check{\nu} * \mu^{*j}(0).$$

Since $\nu * \check{\nu}(0) = \|\nu\|_2^2$ and

$$\mu^{*0}(0) + 2\mu(0) + 3\mu^{*2}(0) + 4\mu^{*3}(0) = 1 + \frac{3}{2d},$$

the $\nu * \check{\nu}(0)$ terms contribute $\|\nu\|_2^2 \left(1 + \frac{3}{2d}\right)$. For $\|a\|_1 = 1$,

$$\mu^{*0}(a) + 2\mu(a) + 3\mu^{*2}(a) + 4\mu^{*3}(a) = \frac{1}{d} + O\left(\frac{1}{d^2}\right), \tag{72}$$

while for $\|a\|_1 > 1$, the sum is $O(d^{-2})$. Thus, for $\nu = \delta_0 - \delta_a$,

$$\nu * \check{\nu} = 2\delta_0 - \delta_a - \delta_{-a} \tag{73}$$

and

$$\|g * \nu\|_2^2 = \frac{2}{4d^2}\left(1 + \frac{3}{2d} - \mathbf{1}(\|a\| = 1)\frac{1}{d} + O\left(\frac{1}{d^2}\right)\right). \tag{74}$$

□

The results obtained by integration are to be compared with the following lower bounds for $\|\xi\|_2^2$ obtained from a convex optimization program.

Lemma 20. *Let $\xi = g * \nu$ be a function on $\mathbb{Z}^d$, $d \geqslant 2$, with reflection antisymmetry in the first k coordinate hyperplanes. Let the corresponding reflection group be $\mathfrak{S}_k$. Consider ξ and ν to be antisymmetric functions on the quotient of $\mathbb{Z}^d/\mathfrak{S}_k$. The following bounds hold for $\|\xi\|_{2,\mathbb{Z}^d/\mathfrak{S}_k}^2$. For all $1 \leqslant i, j \leqslant d$, $i \neq j$,*

$$\|\xi\|_{2,\mathbb{Z}^d/\mathfrak{S}_k}^2 \geqslant \begin{cases} \frac{1}{4d^2+2d} & |\operatorname{supp}\nu| \geqslant 1, \\ \frac{2}{4d^2+6d} & |\operatorname{supp}\nu| \geqslant 2, u, u+e_j \in \operatorname{supp}\nu, \\ \frac{2}{4d^2+2d+1} & |\operatorname{supp}\nu| \geqslant 2, u, u+2e_j \in \operatorname{supp}\nu, \\ \frac{2}{4d^2+2d+2} & |\operatorname{supp}\nu| \geqslant 2, u, u+e_i+e_j \in \operatorname{supp}\nu, \\ \frac{2}{4d^2+2d} & |\operatorname{supp}\nu| \geqslant 2, u, w \in \operatorname{supp}\nu, d(u,w) \geqslant 3. \end{cases} \tag{75}$$

Proof. The optimization program $P'(\{0\}, 1)$ is a lower bound for the first quantity. This program has value $\frac{1}{(2d)(2d+1)}$, since the optimum occurs at an interior point, and is achieved by $x_0 = \frac{1}{2d+1}$, $x_w = \frac{1}{(2d)(2d+1)}$ for $d(w, 0) = 1$.

In the last case, two translated copies of $P'(\{0\}, 1)$ may be applied, one at each point in the support.

In the remaining cases, a lower bound for $\|\xi\|^2_{2,\mathbb{Z}^d/\mathfrak{S}_k}$ is given by setting, for $u = e_1, 2e_1, e_1+e_2$, $\nu_0 = \nu_u = 1$, and calculating $P'(\{0,u\},1)$. The optimum in this case is achieved at an interior point since the values on the boundary are at least $\frac{1}{4}$, which exceeds the claimed bound. At an interior point, by Lagrange multipliers the optimum takes the form

$$x = \lambda_1 v_1 + \lambda_2 v_2, \tag{76}$$

where v_1 and v_2 are the gradients of the two linear constraints. The linear system $v_1^t(\lambda_1 v_1 + \lambda_2 v_2) = 1$, $v_2^t(\lambda_1 v_1 + \lambda_2 v_2) = 1$ is symmetric in λ_1, λ_2 and has a unique solution with $\lambda = \lambda_1 = \lambda_2 = \frac{1}{\|v_1\|_2^2 + v_1^t v_2}$. Thus

$$\|x\|_2^2 = 2\lambda^2(\|v_1\|_2^2 + v_1^t v_2) = \frac{2}{\|v_1\|_2^2 + v_1^t v_2}. \tag{77}$$

Since $\|v_1\|_2^2 = 4d^2 + 2d$ and $v_1^t v_2$ has value $4d, 1, 2$ in the three cases considered, the claim follows. □

Lemma 21. *Let $\xi = g * \nu$ be a function on $\mathbb{Z}^d$, $d \geqslant 5$, satisfying $|\operatorname{supp}\nu| \geqslant 3$. Then*

$$\|\xi\|_2^2 \geqslant \frac{3}{4d^2 + 10d}. \tag{78}$$

Proof. After translation, suppose that $0, u_1, u_2$ are in the support. A lower bound for the 2-norm is given by the value of the optimization program $P'(\{0,u_1,u_2\},1)$:

$$\begin{aligned} \text{minimize:} \quad & \sum_{d(w,\{0,u_1,u_2\})\leqslant 1} x_w^2, \\ \text{subject to:} \quad & 2dx_0 + \sum_{i=1}^d x_{e_i} + x_{-e_i} \geqslant 1, \\ & 2dx_{u_1} + \sum_{i=1}^d x_{u_1+e_i} + x_{u_1-e_i} \geqslant 1, \\ & 2dx_{u_2} + \sum_{i=1}^d x_{u_2+e_i} + x_{u_2-e_i} \geqslant 1. \end{aligned}$$

Let x be the set of variables, and write the constraints as $v_1^t x \geqslant 1$, $v_2^t x \geqslant 1$, $v_3^t x \geqslant 1$. By Lagrange multipliers, the optimum occurs at $x = \lambda_1 v_1 + \lambda_2 v_2 + \lambda_3 v_3$. Since the distance 1 neighborhoods of $0, u_1, u_2$ pairwise overlap in at most 2 points, each neighborhood has some variable not shared by the others. Since the optimum occurs with all variables nonnegative, $\lambda_1, \lambda_2, \lambda_3 \geqslant 0$.

We have $\|v_i\|_2^2 = 4d^2 + 2d$, and for $i \neq j$, $v_i^t v_j \leqslant 4d$. Adding the three constraints,

$$(v_1^t + v_2^t + v_3^t)(\lambda_1 v_1 + \lambda_2 v_2 + \lambda_3 v_3) \geqslant 3. \tag{79}$$

Hence $(\lambda_1+\lambda_2+\lambda_3)\geqslant\frac{3}{4d^2+10d}$, since

$$\begin{aligned}\|x\|_2^2 &= \left(\lambda_1 v_1^t+\lambda_2 v_2^t+\lambda_3 v_3^t\right)(\lambda_1 v_1+\lambda_2 v_2+\lambda_3 v_3)\\ &\geqslant \lambda_1 v_1^t(\lambda_1 v_1+\lambda_2 v_2+\lambda_3 v_3)+\lambda_2 v_2^t(\lambda_1 v_1+\lambda_2 v_2+\lambda_3 v_3)\\ &\quad +\lambda_3 v_3^t(\lambda_1 v_1+\lambda_2 v_2+\lambda_3 v_3)\\ &\geqslant \lambda_1+\lambda_2+\lambda_3\\ &\geqslant \frac{3}{4d^2+10d}.\end{aligned}$$

□

Combining the estimates, it is now possible to prove Theorem 3.

Proof of Theorem 3. In determining $\gamma_{\mathbb{Z}^d}$, $\nu=\Delta\xi$ is C^1, and hence $|\operatorname{supp}\nu|\geqslant 2$. Using $1-c(\xi_x)=2\pi^2\xi_x^2+O(\xi_x^4)$ it follows that $f(\xi)=2\pi^2\|\xi\|_2^2+O(\|\xi\|_2^4)$. By Lemma 21, if $|\operatorname{supp}\nu|\geqslant 3$, then $\|\xi\|_2^2\geqslant\frac{3}{4d^2+10d}$. Combining with Lemma 19, for all d sufficiently large the optimum is achieved by $\nu=\delta_0-\delta_{e_1}$ with $\|\xi\|_2^2=\frac{1}{2d^2}\left(1+\frac{1}{2d}+O\left(d^{-2}\right)\right)$. Hence

$$\gamma_{\mathbb{Z}^d}=\frac{\pi^2}{d^2}\left(1+\frac{1}{2d}+O\left(d^{-2}\right)\right). \tag{80}$$

By Lemma 20, it follows that if $|\operatorname{supp}\nu|\geqslant 2$ for the extremal prevector, then $\|g*\nu\|_2^2\geqslant\frac{1}{2d^2}+O(d^{-3})$. Thus, asymptotically in d, the extremum is achieved with ν a point mass. Approximating $1-c(\xi_x)=2\pi^2\xi_x^2+O(\xi_x^4)$, it follows from Lemma 18 that, as $d\to\infty$, for each j,

$$\gamma_{\mathbb{Z}^d,j}=\frac{\pi^2}{2d^2}\left(1+\frac{3}{2d}+O_j(d^{-2})\right), \tag{81}$$

and, uniformly in j, by the first estimate of Lemma 20,

$$\gamma_{\mathbb{Z}^d,j}\geqslant\frac{\pi^2}{2d^2+d}(1+O(d^{-2})). \tag{82}$$

It follows that, for all j,

$$\Gamma_j\leqslant\frac{(d-j)(2d^2+d+O(1))}{\pi^2}, \tag{83}$$

and for each fixed j,

$$\Gamma_j=\frac{(d-j)(2d^2-3d+O_j(1))}{\pi^2}. \tag{84}$$

In particular, $\Gamma=\Gamma_0=\frac{2d^3-3d^2+O(d)}{\pi^2}$ for all d sufficiently large. □

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