Spanning trees in subgraphs of lattices

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1 Introduction

In a graph G, for a subset S of the vertex set, the induced subgraph determined by S has edge set consisting of all edges of G with both endpoints in S. The (edge) boundary, denoted by ∂S consists of all edges containing one endpoint in S and one endpoint not in S.

We consider the combinatorial Laplacian of a graph and an induced subgraph of a graph. Using the classical matrix-tree theorem [8], the number of spanning trees of a graph is proportional to the product of nonzero eigenvalues of the combinatorial Laplacian. We will introduce the zeta function of a graph and derive its relation to the heat kernel and the number of spanning trees of a graph.

In the second part of the paper, we will focus on the special case which involves induced subgraphs of a lattice graph. We will show that for a connected induced subgraph S of a 2-dimensional lattice graph, the number of spanning trees $\tau(S)$ satisfies

$$ce^{c_1\ |S|-c_2|\partial S|} \leq \tau(S) \leq c' e^{c_1\ |S|+c_3\ |\partial S|^2/|S|} \tag{1}$$

where the constants c_1, c_2 and c_3 are universal contants depending only on the host graph but independent of S.

This can be viewed as a discrete analog of the classical results of H. Weyl [10] and McKean and Singer [9]. This paper is organized as follows. In Section 2, we

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state the relationship of the combinatorial Laplacian and the number of spanning trees. In Section 3, we consider the heat kernel and the zeta function of a graph. In Section 4, we focus on the heat kernel of a lattice graph. In Section 5, we prove the main theorem by using the tools defined in preceding sections. For undefined terminology, the reader is referred to [2] and [3].

2 The combinatorial Laplacian and spanning trees

We consider a graph $G = (V, E)$ with vertex set $V = V(G)$ and edge set $E = E(G)$. Let d_v denote the degree of v in G. Here we assume G contains no multiple edges. The combinatorial Laplacian L of G has rows and columns indexed by vertices of G, defined as follows.

$$L(u,v) = \begin{cases} d_v - l_v & \text{if } u = v \\ -1 & \text{if } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

where l_v denotes the number of loops at v.

For a function $f : V \to \mathbb{R}$, we have

$$Lf(v) = \sum_{\substack{u \in V \\ u \sim v}} [f(v) - f(u)].$$

One of the fundamental theorems in combinatorics is the matrix-tree theorem due to Kirchhoff [8] which states that the number of spanning trees in a graph is equal to the determinant of any principal submatrix of the combinatorial Laplacian.

For a graph G, the combinatorial Laplacian has non-negative eigenvalues, $0 = \rho_0 \le \rho_1 \le \ldots \rho_{n-1}$. The number of spanning trees, denoted by $\tau(G)$, can be related to the eigenvalues of L as follows: (A proof can be found in [1]. For completeness, we briefly describe the proof here).

Theorem 1 *For a graph G on n vertices , the number of spanning trees $\tau(G)$ is :*

$$\tau(G) = \frac{1}{n} \prod_{i \ne 0} \rho_i.$$

Proof: Suppose we consider the characteristic polynomial $p(x)$ of the combinatorial Laplacian L.

$$p(x) = det(L - xI).$$

The coefficient of the linear term is exactly

$$-\prod_{i \neq 0} \rho_i.$$

On the other hand, the coefficient of the linear term of $p(x)$ is -1 times the sum of the determinant of n principal submatrix of L obtained by deleting the i-th row and i-th column. By the matrix-tree theorem, the product $\prod_{i\neq 0} \rho_i$ is exactly n times the number of spanning trees of G. □

3 The heat kernel and the zeta function

In a graph G, let S denote a finite connected induced subgraph of G. The combinatorial Laplacian L_S restricted to S is just

$$L_S f(v) = \sum_{\substack{u \in S \\ u \sim v}} [f(v) - f(u)].$$

for a function $f : S \to \mathbb{R}$ and a fixed $v \in S$.

Let k denote the maximum degree of G. For $t \geq 0$, the heat kernel h_t of an induced graph S is defined by

$$\begin{aligned} h_t &= \sum_i e^{-\lambda_i t} P_i \\ &= e^{-tL_S/k} \\ &= I - \frac{t}{k} L_S + \frac{t^2}{2!k^2} L_S^2 - \ldots \end{aligned}$$

where

$$\lambda_i = \frac{\rho_i}{k}$$

and P_i denotes the projection into the eigenspace associated with eigenvalue ρ_i of L_S. In particular, $h_0 = I$, the identity matrix, and h_t satisfies the heat equation

$$\frac{d\ h_t}{d\ t} = -\frac{1}{k} L_S h_t.$$

The trace formula in its most general form is

$$\sum_x h_t(x,x) = \sum_i e^{-\lambda_i t} \tag{2}$$

We define the trace function:

$$Tr\ (h_t) = \sum_i e^{-\lambda_i t}$$

For a connected induced subgraph S, we consider the ζ-function

$$\zeta(s) = \sum_{i \neq 0} \frac{1}{\lambda_i^s}$$

where λ_i ranges over all nonzero eigenvalues of $\frac{1}{k}L_S$.

Therefore we have

$$-\zeta'(0) = \log \prod_{i \neq 0} \lambda_i. \tag{3}$$

where log denotes the natural logarithm.

Here we relate the number of spanning trees to the zeta function of G (also see [7]).

Theorem 2 *For a connected induced subgraph S in a graph G with maximum degree k, the number of spanning trees, denoted by $\tau(G)$, is equal to*

$$\tau(S) = \frac{k^{|S|-1}}{|S|} e^{-\zeta'(0)}.$$

Proof: Using (3) and Theorem 1, we have

$$\begin{aligned} \tau(S) &= \frac{1}{|S|} \prod_{i \neq 0} \rho_i \\ &= \frac{k^{|S|-1}}{|S|} \prod_{i \neq 0} \lambda_i \\ &= \frac{k^{|S|-1}}{|S|} e^{-\zeta'(0)}. \end{aligned}$$

□

We consider

$$Tr^*(h_t) = \sum_{i\neq 0} e^{-\lambda_i t}.$$

Because of the fact that

$$\int_0^\infty e^{-\lambda t} t^{z-1} dt = \frac{\Gamma(z)}{\lambda^z}$$

we have the following:

Theorem 3

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} Tr^*(h_t) dt \tag{4}$$

We note that we also have the following Mellin inversion formula:

$$Tr^*(h_t) = \frac{1}{2\pi i} \int t^{-s}\Gamma(s)\zeta(s) ds$$

4 The heat kernel for a path

For the one-dimensional case, in an infinite path P, the vertices are labeled by integers and x is adjacent to $x+1$ and $x-1$. The heat kernel of P has been examined in [6] and here we state some facts that will be useful later.

The heat kernel H_t of P satisfies:

$$\begin{aligned} H_t(x,x) &= \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} e^{-t\lambda_j} \\ &= \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} e^{-t(1-\cos\frac{2\pi j}{n})} \\ &= \frac{2}{\pi} \int_0^{\pi/2} e^{-2t\sin^2 y} dy \end{aligned} \tag{5}$$

In general, the heat kernel $H_t(x,y)$ of an infinite path satisfies

$$\begin{aligned} H_t(x,x+a) &= \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} e^{-t\lambda_j} e^{\frac{2\pi i j a}{n}} \\ &= \frac{2}{\pi} \int_0^{\pi/2} e^{-2t\sin^2 y + 2iay} dy \\ &= \frac{2}{\pi} \int_0^{\pi/2} e^{-2t\sin^2 y} \cos 2ay dy \end{aligned} \tag{6}$$

We also need the following fact (see [6]):

$$
\begin{aligned}
H_t(x, x+a) &= H_t(x, x-a) \\
&= (-1)^a e^{-t} \sum_{k \ge a} \frac{\binom{2k}{k+a}}{k!} (\frac{-t}{2})^k \\
&= e^{-t} \sum_{k \ge a} \frac{\binom{a+2k}{k}}{k!} (\frac{t}{2})^{a+2k}
\end{aligned}
$$

The above equality can be used to show the following:

$$
\begin{aligned}
\sum_{a \in \mathbb{Z}^+} H_t(0, 2a+1) &= \frac{1}{2} \sum_{a\ odd} H_t(0, 2a+1) \\
&= \frac{1}{2} e^{-t} \sum_{k\ odd} \frac{(t)^k}{k!} \\
&= e^{-t} \frac{1}{4} (e^{t/2} - e^{-t/2}) \\
&= \frac{1 - e^{-t}}{4} \qquad (7)
\end{aligned}
$$

□

We will also use the following facts [2]:

$$
\begin{aligned}
\frac{d}{d\ t} H_t(x, y) &= -\frac{1}{2} L H_t(x, y) \qquad (8) \\
&= -\frac{1}{2} \sum_{x' \sim x} (H_t(x, y) - H_t(x', y)). \qquad (9)
\end{aligned}
$$

Also, we have

$$
H_0(x, y) = \begin{cases} 1 & \text{if } x = y, \\ 0 & \text{otherwise.} \end{cases}
$$

5 The heat kernel for lattice graphs

In this section, we consider the k-dimensional lattice graphs and their induced subgraphs. We define the lattice graph $P_n^{(r)}$ to be the cartesian product of k copies of an n-cycle. The infinite lattice graph $P^{(k)}$ is just by taking the limit of $P_n^{(r)}$ as n approaches infinity. In particular, for the 2−dimensional lattice graph $p^{(2)}$, each vertex is labelled by $(x, y), x, y \in \mathbb{Z}$. The vertex (x, y) is adjacent to $(x+1, y), (x-1, y), (x, y+1)$ and $(x, y-1)$.

In an infinite 2−dimensional lattice graph $P^{(2)}$, the heat kernel $H_t^{(2)}$ satisfies

$$H_t^{(2)}((x,y),(x+a,y+b)) = H_{t/2}(x,x+a)H_{t/2}(y,y+b) \qquad (10)$$

where H_t is the heat kernel for an infinite path. In general, we have

$$H_t^{(r)}(x,x+a)) = \prod_{i=1}^{r} H_{t/r}(x_i,x_i+a_i) \qquad (11)$$

where $x = (x_1,\ldots,x_r)$.

For certain induced subgraphs of the r−dimensional lattice graphs $P^{(r)}$, we want to derive sharp estimates for the products of the nonzero eigenvalues of the combinatorial Laplacian. To do so, we consider the heat kernel h_t of an induced subgraph S of $P^{(r)}$. From (4), we have

$$\begin{aligned}\zeta(s) &= \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1} Tr^*\ h_t dt \\ &= \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}(\sum_{x\in S} h_t(x,x)-1)dt\end{aligned}$$

Of particular interest are subgraphs S whose trace can be estimated by using the heat kernel of the lattice graph $P^{(r)}$. We define the function ζ_0 as follows:

$$\zeta_0(s) = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1} H_t^{(r)}(x,x)dt$$

Using (5) and (11), we have

$$\begin{aligned}\zeta_0(s) &= \frac{1}{\Gamma(s)}(\frac{2}{\pi})^r \int_0^{\pi/2}\cdots\int_0^{\pi/2}\int_0^\infty t^{s-1}e^{-2^{2-r}(\sin^2 x_1+\cdots+\sin^2 x_r)}dt dx_1\cdots dx_r \\ &= (\frac{2}{\pi})^r \int_0^{\pi/2}\cdots\int_0^{\pi/2}\frac{1}{(2^{2-r}(\sin^2 x_1+\cdots+\sin^2 x_r))^s}dx_1\cdots dx_r\end{aligned}$$

Therefore we have

$$\zeta_0'(0) = -(\frac{2}{\pi})^r \int_0^{\pi/2}\cdots\int_0^{\pi/2}\log(2^{2-r}(\sin^2 x_1+\cdots+\sin^2 x_r))dx_1\cdots dx_r \qquad (12)$$

In particular, for the case of $r = 2$, we have

$$\begin{aligned}\zeta_0'(0) &= -(\frac{2}{\pi})^2 \int_0^{\pi/2}\int_0^{\pi/2}\log(\sin^2 x+\sin^2 y)dxdy \\ &= 0.220050745\cdots\end{aligned}$$

If h_t can be approximated by $H_t^{(2)}$, then we can derive the following first-order estimate :

$$\tau(S) \approx 4^{|S|-1} e^{-\zeta_0'(0)|S|}$$

This has a similar flavor as the formula of H. Weyl [10] for bounded regions of $\mathbb{R}^k$. To derive such estimates in a precise manner, we will examine the difference of H_t and h_t^* in the next section.

6 The heat kernel of an induced subgraph of the lattice graph

Suppose S is an induced subgraph of the 2-dimensional lattice graph $P^{(2)}$. In order to enumerate the number of spanning trees of S, We will first establish the relation between the heat kernel of S and the heat kernel of $P^{(2)}$.

We start with the combinatorical Laplacian L_S for the induced subgraph S which acts on functions $f : S \to \mathbb{R}$ as follows: For x in S, we have

$$L_S f(x) = \sum_{\substack{y \in S \\ y \sim x}} [f(x) - f(y)]$$

In this section, we denote the heat kernel of S by $h_t(x, y) = h(t, x, y)$ and the heat kernel of $P^{(r)}$ by $H_t^{(2)}(x, y) = \mathbf{H}(t, x, y)$. From the definition, we have

$$\frac{d}{d\,t} h_t = -\frac{1}{4} L_S h_t, \quad \frac{d}{d\,t} \mathbf{H}_t = -\frac{1}{4} L \mathbf{H}_t$$

We consider, for $x, y \in S$,

$$\begin{aligned}
& \int_0^t \frac{d}{d\,s} \sum_{z \in S} h(t-s, x, z) \mathbf{H}(s, z, y) ds \\
= \quad & \sum_{z \in S} [h(0, x, z) \cdot \mathbf{H}(t, z, y) - h(t, x, z) \cdot \mathbf{H}(0, z, y)] \\
= \quad & \mathbf{H}(t, x, y) - h(t, x, y).
\end{aligned}$$

On the other hand, for fixed x and y in S, we have

$$
\begin{aligned}
& \mathbf{H}(t,x,y) - h(t,x,y) \\
= & \int_0^t \frac{d}{d\ s} \sum_{z\in S} h(t-s,x,z)\mathbf{H}(s,z,y)ds \\
= & \int_0^t \sum_{z\in S} (\frac{d}{d\ s} h(t-s,x,z)\cdot \mathbf{H}(s,z,y) + h(t-s,x,z)\cdot \frac{d}{d\ s}\mathbf{H}(s,z,y)]ds \\
= & \int_0^t \sum_{z\in S} \frac{1}{4}\left[L_S h(t-s,x,z)\cdot \mathbf{H}(s,z,y) - h(t-s,x,z)\cdot L\mathbf{H}(s,z,y)\right] ds \\
= & \int_0^t \frac{1}{4}\left[\sum_{\substack{z,w\in S\\ z\sim w}} (h(t-s,x,z) - h(t-s,x,w)(\mathbf{H}(s,z,y) - \mathbf{H}(s,w,y)) - \sum_{z\in S} h(t-s,x,z)\cdot L\mathbf{H}(s,z,y)\right] ds \\
= & -\frac{1}{4}\int_0^t \sum_{\substack{z\in S, z'\notin S\\ z\sim z'}} h(t-s,x,z)[\mathbf{H}(s,z,y) - \mathbf{H}(s,z',y)]ds
\end{aligned}
$$

Thus, we have

$$
h = \mathbf{H} + Q\ h \tag{13}
$$

where Q is defined as follows:

$$
Qh(t,x,y) \quad = \quad \frac{1}{4}\int_0^t \sum_{\substack{z\in S, z'\notin S\\ z\sim z'}} h(t-s,x,z)[\mathbf{H}(s,z,y) - \mathbf{H}(s,z',y)]ds
$$

Thus we have

$$
h = \mathbf{H} + Q\mathbf{H} + Q^2\mathbf{H} + \ldots + Q^{r-1}\mathbf{H} + Q^r h.
$$

We have proved the following:

Theorem 4 *For a connected induced subgraph S in the 2-dimensional lattice graph, the heat kernel h of S satisfies the following:*

$$
h = \mathbf{H} + Q\mathbf{H} + Q^2\mathbf{H} + \ldots + Q^{r-1}\mathbf{H} + Q^r h
$$

where

$$
Qh(t,x,y) \quad = \quad \frac{1}{4}\int_0^t \sum_{\substack{z\in S, z'\notin S\\ z\sim z'}} h(t-s,x,z)[\mathbf{H}(s,z,y) - \mathbf{H}(s,z',y)]ds
$$

As a consequence of Theorem 4, we also have the following useful fact:

Theorem 5 *For a connected induced subgraph S in the 2-dimensional lattice graph, the heat kernel $\mathbf{H}$ of the lattice graph satisfies the following:*

$$1 - \sum_{x\in S} \mathbf{H}(t,x,y) \quad = \quad \frac{1}{4}\int_0^t \sum_{\substack{z\in S, z'\notin S\\ z\sim z'}} [\mathbf{H}(s,z,y) - \mathbf{H}(s,z',y)]ds \tag{14}$$

Proof: The proof follows from Theorem 4 (for the case of $r = 1$) and the fact that

$$\sum_{x\in S} h(t,x,y) = 1.$$

□

Using the definition of Q, (14) can be written as

$$1 \quad = \quad \sum_{x\in S} \mathbf{H}(t,x,y) + Q1(y)$$

and

$$1 \quad = \quad \frac{1}{|S|}\sum_{x,y\in S} (\mathbf{H}(t,x,y) + Q\mathbf{H}(t,x,y) + \ldots + Q^k\mathbf{H}(t,x,y)) + Q^{k+1}1$$

where

$$Q^k 1 = \frac{1}{|S|}\sum_{y\in S} Q^k 1(y).$$

7 The heat kernel of a half plane

In this section, we consider a special induced subgraph of the 2-dimensional lattice graph $P^{(2)}$. First, we consider a *half plane* F which is an induced subgraph of $P^{(2)}$ with vertex set $\{v = (a,b) : a \geq 0\}$.

We remark that from the definition of the combinatorial Laplacian in Section 2, we see that for a graph G and a graph G' that is resulted by adding a loop to G, their combinatorial Laplacians are identical. An induced subgraph S of a regular graph is not regular in general. We will often consider adding loops to vertices of S which are adjacent to vertices not in S so that all the degrees are equal in the resulting graph. The closure of an induced subgraph S, denoted by $\hat{S}$, is by adding p loops to every vertex v in S which is incident to p edges in the edge boundary ∂S. Clearly, the closure of an induced subgraphs have the same heat kernel.

Our goal is to express the heat kernel of a half plane in terms of the heat kernel of $P^{(2)}$.

Theorem 6 *The heat kernel $\bar{h}$ of the halfplane F satisfies, for vertices u and u of F,*

$$\bar{h}(t,u,v) = \mathbf{H}(t,u,v) + \mathbf{H}(t,u,\bar{v})$$

where $\bar{v}$ is the mirrow image of the vertex v with respect to the line $x = -1/2$.

Proof: We note that

$$\bar{h}(t,u,v) = e^{-t} \sum_{r \geq 0} w_r(u,v) \frac{t^r}{r!}$$

where $w_r(u,v)$ denote the number of walks of length r from u to v in the closure the half plane F. It suffices to show that we can have $w_r(u,v) = w'_r(u,v) + w"_r(u,\bar{v})$ where $w'_r(u,v)$ is the number of walks of length r from u to v in $P^{(2)}$ and $w"_r(u,\bar{v})$ is the number of walks of length r from u to $\bar{v}$ in $P^{(2)}$.

We observe that a walk in the plane $P^{(2)}$ joining u to v corresponds to a walk in $\hat{F}$ by reflecting using the line $x = -1/2$. Namely, a walk which visits $\bar{v} \notin F$ shall be mapped to the corresponding walk which visit $v \in F$. Furthermore, an edge from v which crosses the line $x = -1/2$ is corresponding to a loop at v. A walk of length r from u to v in $P^{(2)}$ is then mapped to a walk of the same length from v to v in $\hat{F}$ with an even number of loops. Also, a walk of length r from u to v in $\hat{F}$ which contains an odd number of loops is mapped to walks of length r from u to $\bar{v}$ in $P^{(2)}$. In fact, such correspondences give a bijection. Therefore, we have

$$\bar{h}(t,u,v) = \mathbf{H}(t,u,v) + \mathbf{H}(t,u,\bar{v}).$$

□

We now define another operator $\mathbf{Q}$ as follows:

$$\mathbf{Q}h(t,u,v) \quad = \quad \frac{1}{4}\int_0^t \sum_{\substack{z\in F, z'\notin F\\ z\sim z'}} h(t-s,u,z)[\mathbf{H}(s,z,v)-\mathbf{H}(s,z',v)]ds \qquad (15)$$

Theorem 7 *For two vertices x and y in he half plane F, we have*

$$\mathbf{H}(t,u,\bar{v}) = \mathbf{QH}(t,u,v) + \mathbf{Q}^2\mathbf{H}(t,u,v) + \ldots$$

where $\bar{v}$ is the mirrow image of the vertex v with respect to the line $x=-1/2$.

Proof: The proof follows from Theorem 6, which says

$$\bar{h}(t,x,y) - \mathbf{H}(t,x,y) = \mathbf{H}(t,x,\bar{y}).$$

Then we use Theorem 4 which states that

$$\bar{h}(t,x,y) - \mathbf{H}(t,x,y) = \mathbf{QH}(t,x,y) + \mathbf{Q}^2\mathbf{H}(t,x,y) + \ldots .$$

□

Another consequence of (15) is the following:

Theorem 8

$$\sum_{\substack{a\in\mathbb{Z}^+\\ v=(a,0)}} \mathbf{Q}f(t,v,v) \quad = \quad \frac{1}{4}\int_0^t \sum_{x\in F} f(t-s,x,z_0)[\mathbf{H}(s,z_0,v)-\mathbf{H}(s,z_0',x)]ds$$

for $z_0=(0,0), z_0'=(-1,0)$ and for any f.

Proof: We sum (15) over all vertices v in F.

$$\begin{aligned}\sum_{\substack{a\in\mathbb{Z}^+\\ v=(a,0)}} \mathbf{Q}f(t,v,v) &= \frac{1}{4}\int_0^t \sum_{\substack{a\in\mathbb{Z}^+\\ v=(a,0)}} \sum_{\substack{z\in F, z'\notin F\\ z\sim z'}} f(t-s,v,z)[\mathbf{H}(s,z,v)-\mathbf{H}(s,z',v)]ds \\ &= \frac{1}{4}\int_0^t \sum_{x\in F} f(t-s,x,z)[\mathbf{H}(s,z_0,v)-\mathbf{H}(s,z_0',x)]ds\end{aligned}$$

□

8 Bounding the number of spanning trees

Suppose S is an induced subgraph of the 2-dimensional lattice graph $P^{(2)}$. We will prove the main theorem.

Theorem 9 *For a connected induced subgraph S in the 2-dimensional lattice graph, the number of spanning trees $\tau(S)$ of S satisfies:*

$$\frac{1}{|S|}(4e^{-\alpha})^{|S|-1}e^{-\beta|\partial S|(1-1/|S|)} \leq \tau(S) \leq \frac{1}{|S|}4^{|S|-1}e^{-\alpha(|S|-|\partial S|^2/|S|)}$$

where

$$\begin{aligned}
\alpha &= -(\frac{2}{\pi})^2\int_0^{\pi/2}\int_0^{\pi/2}\log((\sin^2 x_1+\sin^2 x_2))dx_1dx_2 \\
&\approx .2200507\ldots \\
\beta &= -\frac{1}{2\pi}\int_0^{\pi/2}(\log\sin^2 x - \log(1+\sin^2 x))dx \\
&\approx .44068679...
\end{aligned}$$

Proof: From Theorem 4, we have

$$h = \mathbf{H} + Q\mathbf{H} + Q^2\mathbf{H} + \ldots + Q^{r-1}\mathbf{H} + Q^r h.$$

We consider the trace of h. For simplicity, we write

$$Tr_S\mathbf{H}_t = \sum_{x\in S} Q\mathbf{H}(t,x,x).$$

We have

$$\begin{aligned}
Tr_S Q\mathbf{H}_t &= \sum_{x\in S} Q\mathbf{H}_t(x,x) \\
&= \sum_{\substack{z\in S, z'\notin S\\ z\sim z'}} \frac{1}{4}\sum_{x\in S}\int_0^t \mathbf{H}(t-s,x,z)[\mathbf{H}(s,z,x)-\mathbf{H}(s,z',x)]ds \\
&\leq \sum_{\substack{z\in S, z'\notin S\\ z\sim z'}} \frac{1}{4}\sum_{x\in F_z}\int_0^t \mathbf{H}(t-s,x,z)[\mathbf{H}(s,z,x)-\mathbf{H}(s,z',x)]ds
\end{aligned}$$

where F_z is the half plane consisting of all points closer to z than to z'. Thus, we have

$$Tr_S Q\mathbf{H}_t \leq \frac{|\partial S|}{4}\sum_{x\in F_z}\int_0^t \mathbf{H}(t-s,x,z)[\mathbf{H}(s,z,x)-\mathbf{H}(s,z',x)]ds$$

Using Theorem 8, we get

$$\begin{aligned} Tr_S Q\mathbf{H}_t &= \sum_{x\in S} Q\mathbf{H}(t,x,x) \\ &\leq |\partial S| \sum_{\substack{a\in\mathbb{Z}^+ \\ v=(a,0)}} \mathbf{QH}(t,v,v) \end{aligned}$$

By repeatedly using Theorem 8, we have

$$\begin{aligned} Tr_S Q^j\mathbf{H}_t &= \sum_{x\in S} Q^j\mathbf{H}(t,x,x) \\ &\leq |\partial S| \sum_{\substack{a\in\mathbb{Z}^+ \\ v=(a,0)}} \mathbf{Q}^j\mathbf{H}(t,v,v) \end{aligned}$$

Summing over j, we have

$$\begin{aligned} \sum_{j\geq 1} Tr_S Q^j\mathbf{H}_t &\leq |\partial S| \sum_{\substack{a\in\mathbb{Z}^+ \\ v=(a,0)}} \sum_{j\geq 1} \mathbf{Q}^j\mathbf{H}(t,v,v) \\ &= |\partial S| \sum_{\substack{a\in\mathbb{Z}^+ \\ v=(a,0)}} \mathbf{H}(t,v,\bar{v}) \qquad (16) \end{aligned}$$

by using Theorem 7.

Then we have

$$\begin{aligned} \zeta(s) &= \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}(Tr(h_t)-1)dt \\ &= \frac{|S|}{\Gamma(s)}\int_0^\infty t^{s-1}\mathbf{H}(t,x,x)dt + \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}(Tr_S Q\mathbf{H}_t + \ldots + TrQ^r\mathbf{H}_t) \\ &\quad -\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}(1-Q^{r+1}1)dt \\ &= \zeta_0(s)|S| + \zeta_1(s) + \zeta_2(s) \end{aligned}$$

From the previous section, we know that

$$\begin{aligned} \zeta_0'(0) &= -(\frac{2}{\pi})^2 \int_0^{\pi/2}\int_0^{\pi/2} \log(\sin^2 x + \sin^2 y)dxdy \\ &= 0.220050745\cdots \end{aligned}$$

It suffices to estimate and bound $\zeta_1'(0)$ and $\zeta_2'(0)$. We will use the fact that for differentiable functions f, g with $f(0) = g(0)$, if $f(x) \leq g(x)$ for $x \geq 0$, then $f'(0) \geq g'(0)$.

$$\begin{aligned}
\zeta_1(s) &\leq \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\ (Tr_S\ Q\mathbf{H}_t+\dots)\ dt \\
&\leq \frac{|\partial S|}{\Gamma(s)}\int_0^\infty t^{s-1}\sum_{\substack{a\in\mathbb{Z}^+\\ v=(a,0)}}\mathbf{H}(t,v,\bar{v})dt \\
&= \frac{|\partial S|}{4\Gamma(s)}\int_0^\infty t^{s-1}\ (1-e^{-t})H(t/2,0,0)dt
\end{aligned}$$

by using (7). Therefore we have

$$\begin{aligned}
\zeta_1(s) &\leq \frac{|\partial S|}{4\Gamma(s)}\int_0^\infty t^{s-1}(1-e^{-t})\frac{2}{\pi}\int_0^{\pi/2} e^{-t\sin^2 x}dxdt \\
&= \frac{|\partial S|}{2\pi}\int_0^{\pi/2}\left(\frac{1}{\sin^{2s}x}-\frac{1}{(1+\sin^2 x)^s}\right)dx
\end{aligned}$$

Consequently,

$$\begin{aligned}
\zeta_1'(0) &\leq -\frac{|\partial S|}{2\pi}\int_0^{\pi/2}(\log\sin^2 x-\log(1+\sin^2 x))dx \\
&= \beta|\partial S| \\
&\approx .44068679...|\partial S| \qquad (17)
\end{aligned}$$

It remains to bound ζ_2. From Theorem 4, we see that for any $x\in S$,

$$1-Q^{r+1}1(x)=\sum_{y\in S}\mathbf{H}(x,y)+\sum_{j=1}^{r}\sum_{y\in S}Q^j\mathbf{H}(t,x,y).$$

We also note that for $x\neq y$,

$$\lim_{s\to 0}\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\mathbf{H}(t,x,y)dt=0$$

In fact, we have, in general,

$$\lim_{s\to 0}\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}Q^j\mathbf{H}(t,x,y)dt=0$$

Therefore we have

$$\lim_{s\to 0}\zeta_2(0)=\frac{1}{n}(\zeta_0(0)+\zeta_1(0))$$

Clearly, we have

$$\begin{aligned}
\zeta_2(x) &\leq -\frac{1}{\Gamma(s)}\int_0^\infty \sum_{j\geq 0}\sum_{x,y}\mathbf{H}(t,x,y)dt \\
&\leq -\frac{1}{|S|}(\zeta_0(0)+\zeta_1(0)) - \frac{1}{\Gamma(s)}\int_0^\infty \sum_{j\geq 0}\sum_{x\neq y}\mathbf{H}(t,x,y)dt \\
&\leq -\frac{1}{|S|}(\zeta_0(0)|S|+\zeta_1(0)).
\end{aligned}$$

Altogether, we have

$$\zeta'(0) \leq \alpha(|S|-1) + \beta|\partial S|(1-\frac{1}{|S|}).$$

This implies

$$\tau(S) \geq \frac{1}{|S|}(4e^{-\alpha})^{|S|-1}e^{-\beta|\partial S|(1-1/|S|)}.$$

To upper bound $\tau(S)$, it is enough to lower bound $\zeta'(0)$. We consider

$$\begin{aligned}
\zeta(s) &= \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}(Tr(h_t)-1)dt \\
&\geq \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}(\sum_{x\in S}\mathbf{H}(t,x,x) - \frac{1}{|S|}\sum_{x,y\in S}\mathbf{H}(t,x,y))dt \\
&\quad + \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}(\sum_{r\geq 1}\sum_{x\in S}Q^r\mathbf{H}(t,x,x) - \frac{1}{|S|}\sum_{x,y\in S}Q^r\mathbf{H}(t,x,y))dt \\
&\geq \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\sum_{x\in S}\mathbf{H}(t,x,x) - \frac{1}{|S|}\sum_{x,y\in S}\mathbf{H}(t,x,y)dt \\
&= |S|\zeta_0(s)+\zeta_3(s)
\end{aligned}$$

where

$$\zeta_3(s) = -\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\frac{1}{|S|}\sum_{x,y\in S}\mathbf{H}(t,x,y)dt$$

We consider

$$F(t) = \sum_{x,y\in S}\mathbf{H}(t,x,y) - |\partial S|^2\mathbf{H}(t,x,x).$$

We note that

$$\begin{aligned}
\frac{d}{d\,t}F(t) &= -\sum_{x\in S}\sum_{y\in S}\frac{1}{4}LH(t,x,y) + \frac{|\partial S|^2}{4}L\mathbf{H}(t,x,x) \\
&= -\frac{1}{4}\sum_{x\in S}\sum_{\substack{y\in S, y'\notin S\\ y\sim y'}}(\mathbf{H}(t,x,y)-\mathbf{H}(t,x,y')) + \frac{|\partial S|^2}{4}L\mathbf{H}(t,x,x)
\end{aligned}$$

and

$$\begin{aligned}
\frac{d^2}{d\,t^2}F(t) &= -\frac{1}{16}\sum_{\substack{x\in S, x'\notin S\\ x\sim x'}}\sum_{\substack{y\in S, y'\notin S\\ y\sim y'}}(\mathbf{H}(t,x,y)-\mathbf{H}(t,x,y')-(\mathbf{H}(t,x',y)-\mathbf{H}(t,x',y'))\\
&\quad -\frac{|\partial S|^2}{16}L^2\mathbf{H}(t,x,x)\\
&\le 0
\end{aligned}$$

Therefore, we have

$$\frac{d}{d\,t}F(t)\le \lim_{t\to\infty}\frac{d}{d\,t}F(t)=0.$$

Consequently,

$$F(t)\le \lim_{t\to\infty}F(t)=0$$

and

$$\sum_{x,y\in S}\mathbf{H}(t,x,y)dt\le |\partial S|^2\mathbf{H}(t,x,x).$$

This implies

$$\begin{aligned}
\zeta_3(s) &= -\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\frac{1}{|S|}\sum_{x,y\in S}\mathbf{H}(t,x,y)dt\\
&\ge -\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\frac{|\partial S|^2}{|S|}\mathbf{H}(t,x,x)dt\\
&\ge -\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\frac{|\partial S|^2}{|S|}\mathbf{H}(t,x,x)dt
\end{aligned}$$

Therefore we have

$$\zeta_3(s)\ge= -\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\frac{|\partial S|^2}{|S|}\mathbf{H}(t,x,x)dx$$

and

$$\zeta_3'(0)\quad\ge\quad -\frac{|\partial S|^2}{|S|}\alpha$$

Therefore

$$\tau(S)\le\frac{1}{|S|}4^{|S|-1}e^{-\alpha(|S|-|\partial S|^2/|S|)}.$$

This completes the proof of Theorem 3.

We remark that the various constants in Theorem 9 can be improved by imposing additional conditions on the induced subgraph S. For example, suppose that the induced subgraph S consists of vertices within an area with boundary consisting of horizontal and vertical line segments. If the boundary line segments are large, we can derive sharper estimates for $\zeta'(0)$. In additional, various convexity conditions [4, 5] can be explored. However, these further considerations will not be included here.

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