

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

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

where the constants c_1 , c_2 and c_3 are universal constants 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 $f : V \rightarrow \mathbb{R}$, 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, $0 = \rho_0 \leq \rho_1 \leq \dots \leq \rho_{n-1}$. 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 :*

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

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 . \square

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 $f : S \rightarrow \mathbb{R}$ 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

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

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

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

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

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

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

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

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:

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

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

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

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

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

The above equality can be used to show the following:

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

□

We will also use the following facts [2]:

$$\frac{d}{dt} H_t(x, y) = -\frac{1}{2} L H_t(x, y) \tag{8}$$

$$= -\frac{1}{2} \sum_{x' \sim x} (H_t(x, y) - H_t(x', y)). \tag{9}$$

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

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

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

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

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

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

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

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

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

Therefore we have

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

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

$$\begin{aligned} \zeta_0'(0) &= -\left(\frac{2}{\pi}\right)^2 \int_0^{\pi/2} \int_0^{\pi/2} \log(\sin^2 x + \sin^2 y) dx dy \\ &= 0.220050745 \dots \end{aligned}$$

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 combinatorial Laplacian L_S for the induced subgraph S which acts on functions $f : S \rightarrow \mathbb{R}$ 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

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

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

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

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

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

Thus, we have

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

where Q is defined as follows:

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

Thus we have

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

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:*

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

where

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

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:*

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

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

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

and

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

where

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

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:

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

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

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

where \bar{v} is the mirror 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

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

□

Another consequence of (15) is the following:

Theorem 8

$$\sum_{\substack{a \in \mathbb{Z}^+ \\ v=(a,0)}} \mathbf{Q}f(t, v, v) = \frac{1}{4} \int_0^t \sum_{x \in F} f(t-s, x, z_0) [\mathbf{H}(s, z_0, v) - \mathbf{H}(s, z'_0, x)] ds$$

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

$$\begin{aligned} \alpha &= -\left(\frac{2}{\pi}\right)^2 \int_0^{\pi/2} \int_0^{\pi/2} \log((\sin^2 x_1 + \sin^2 x_2)) dx_1 dx_2 \\ &\approx .2200507 \dots \\ \beta &= -\frac{1}{2\pi} \int_0^{\pi/2} (\log \sin^2 x - \log(1 + \sin^2 x)) dx \\ &\approx .44068679 \dots \end{aligned}$$

Proof: From Theorem 4, we have

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

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

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

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

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

by using Theorem 7.

Then we have

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

From the previous section, we know that

$$\begin{aligned} \zeta'_0(0) &= -\left(\frac{2}{\pi}\right)^2 \int_0^{\pi/2} \int_0^{\pi/2} \log(\sin^2 x + \sin^2 y) dx dy \\ &= 0.220050745 \dots \end{aligned}$$

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

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

Consequently,

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

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 $x \neq y$,

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

In fact, we have, in general,

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

Therefore we have

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

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

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

and

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

Therefore, we have

$$\frac{d}{d t} F(t) \leq \lim_{t \rightarrow \infty} \frac{d}{d t} F(t) = 0.$$

Consequently,

$$F(t) \leq \lim_{t \rightarrow \infty} F(t) = 0$$

and

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

This implies

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

Therefore we have

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

and

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

Therefore

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

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 addition, various convexity conditions [4, 5] can be explored. However, these further considerations will not be included here.

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