HEAT KERNELS ON FORMS DEFINED ON A SUBGRAPH OF A COMPLETE GRAPH

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Abstract. We study the heat kernel expansion of the Laplacian on n-forms defined on a subgraph of a directed complete graph. We derive two expressions for the subgraph heat kernel on 0-forms and compute the coefficients of the expansion. We also obtain the subgraph heat kernel of the Laplacian on 1-forms.

1. Introduction

Given a directed complete graph K and a subgraph G, one can define n-forms on both G and K as well as Laplacians on these forms (see e.g., [6, 7]). The main purpose of this paper is to derive formulas for the the heat kernel expansion for the Laplacian on n-forms on G in terms of the heat kernel of the Laplacian on n-form on K. This has an analog in Riemannian geometry, with K playing the role of the Euclidean space $\mathbb{R}^n$ and G playing the role of an n-dimensional Riemannian manifold. Spectral graph theory and heat heat kernels on graphs have been studied by many authors (see [3] and the references therein). In general, it is not easy to compute the heat kernel on graphs. Nevertheless, Chung and Yau [4, 5] derived formulas for the heat kernel on lattice graphs, n-cycles, k-regular graphs, and the k-tree. Grigor'yan and Telcs [8] obtained conditions under which a two-sided sub-Gaussian heat kernel estimate for a weighted graph holds. More recently, Chinta *et al.* [2] derived a formula for the heat kernel on regular trees in terms of the classical I-Bessel functions.

This paper studies heat kernels on subgraphs. In addition to functions on the graphs and subgraphs, we also study forms on them. In the classical setting, the heat kernels on forms yields interesting geometric information, such as the Euler characteristic and the Gauss-Bonnet Theorem (see [11, 14]). For non-directed graphs, the Gauss-Bonnet Theorem and Mckean-Singer Theorem on the Euler characteristic have been studied by Knill [9, 10]. In this paper, we consider directed graphs. We start by deriving a formal expression for the heat kernel of the Laplacian on n-forms on a subgraph in terms of a geometric series of an operator and the heat kernel on n-forms defined

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on the entire graph, namely,

$$H_t^G(x,y) = \Big(\sum_{m=0}^{\infty} T^m\Big) H_t^K(x,y), \tag{1.1}$$

where T is some linear operator. See Theorem 2.4 in Section 2.

For 0-forms, i.e., functions defined on K, the terms $T^m H_t^K$ in (1.1) can be computed explicitly in terms of the difference of the Laplacians $\Delta^{G^c} := \Delta^K - \Delta^G$, where Δ^K and Δ^G are the combinatorial Laplacians on K and G respectively. This allows us to derive a formula for $H_t^G(x,y)$ and express it in three different forms. See Theorem 3.4, Corollary 3.4, and Corollary 3.7 in Section 3.

Section 4 is devoted to computing the coefficients of the subgraph heat kernel expansion obtained in Section 3.

In Section 5, we use another method to obtain the expansion of the heat kernel on a subgraph of a complete graph. This method was first introduced by Minakshisundaram-Pleijel and then used by Minakshisundaram to construct the heat kernel on compact Riemannian manifolds (see [1, 12, 13]), which has the form:

$$\frac{1}{(4\pi t)^{n/2}} e^{-d(x,y)^2/(4t)} \big(u_0(x,y) + u_1(x,y)t + \cdots + u_k(x,y)t^k + \cdots\big).$$

We compute explicit formulas for the functions that are analogs of $u_i(x,y)$, $i = 0,1,2$ (see Proposition 5.1). The terms in the series expansion of a subgraph heat kernel obtained by the two different methods appear in quite different forms. We verify that the first few terms of the two series expansions agree.

For n forms it is in general not clear how $T^m H_t^K(x,y)$ can be computed explicitly. Nevertheless, we show Section 6 that by solving a system of ODEs, one can derive an explicit formula for the heat kernel on a 1-forms on a complete graph, and use it to obtain an expression for $H_t^G(x,y)$.

2. Recursive formula for heat kernels on n-forms of a subgraph

Let $K = K_N$ be the complete graph with N vertices. Let $V_0 := \{1, 2, \ldots, N\}$ denote the set of vertices. For $n \geq 1$, let

$$V_n := \{i_0 \cdots i_n : i_0, \ldots, i_n \in V_0, i_j \neq i_{j+1} \text{ for all } j = 0, \ldots, n-1\}$$

denote the set of directed paths of length $n+1$. Let G be a subgraph of K with vertex set $V_0^G \subseteq V_0$ and edge set $V_1^G \subseteq V_1$. For $n \geq 1$, let

$$V_n^G := \{i_1 \cdots i_n \in V_n : i_j i_{j+1} \in V_0^G \text{ for all } j = 1, \ldots, n-1\}$$

denote the set of directed paths in the graph G.

We let G^c be the complement of G defined as follows. Let $V_0^{G^c} := V_0 \setminus V_0^G$ and call it the set of vertices of G^c. Let $V_1^{G^c} := V_1 \setminus V_1^G$. Note that G^c is not necessarily a graph, since an edge in $V_1^{G^c}$

does not necessarily connect two vertices in $V_0^{G^c}$. In fact, in Example 2.1 below, G^c has vertex set $V_0^{G^c} = \{3\}$ and edge set $V_1^{G^c} = \{13, 23, 31, 32\}$ and thus it is not a graph. For each $n \geq 1$, let

$$V_n^{G^c} := V_n \setminus V_n^G \tag{2.1}$$

be the set of directed paths of length $n+1$ associated with G^c. Note that a directed path in $V_n^{G^c}$ may contain a subpath that belongs to some V_k^G, $1 \leq k \leq n-1$. For instance, in Example 2.1 below, the path $123 \in V_2^{G^c}$ contains the subpath 12 that belongs to V_1^G.

For each $n \geq 0$, we call any real-valued function on V_n an *n-form* on V_n, and let Λ^n be the vector space of all n-forms on V_n. Let $\{e^{i_0\cdots i_n}\}_{i_0\cdots i_n \in V_n}$ be the canonical basis on Λ^n with $e^{i_0\cdots i_n}$ taking the value 1 at $i_0 \cdots i_n$ and zero elsewhere. Define the *exterior operator* $d_n = d_n^K : \Lambda^n \to \Lambda^{n+1}$ as follows. For

$$\omega = \sum_{i_0\cdots i_n \in V_n} \omega_{i_0\cdots i_n} e^{i_0\cdots i_n} \in V_n, \tag{2.2}$$

define

$$(d_n\omega)_{i_0\cdots i_{n+1}} := \sum_{k=0}^{n+1} (-1)^k \omega_{i_0\cdots \hat{i}_k \cdots i_{n+1}},$$

where $\hat{i}_k$ means that the index i_k is removed. For each $n \geq 0$, we also define d_n^G and $d_n^{G^c}$ as follows. Let ω be as in (2.2). Then

$$d_n^G(\omega) := \sum_{i_0\cdots i_n \in V_n} \omega_{i_0\cdots i_n} d_n^G(e^{i_0\cdots i_n}),$$

where

$$d_n^G(e^{i_0\cdots i_n}) := \begin{cases} d_n(e^{i_0\cdots i_n}) & \text{if } i_0 \cdots i_n \in V_n^G, \\ 0 & \text{otherwise.} \end{cases} \tag{2.3}$$

Similarly, define

$$d_n^{G^c}(\omega) := \sum_{i_0\cdots i_n \in V_n} \omega_{i_0\cdots i_n} d_n^{G^c}(e^{i_0\cdots i_n}),$$

where

$$d_n^{G^c}(e^{i_0\cdots i_n}) := \begin{cases} d_n(e^{i_0\cdots i_n}) & \text{if } i_0 \cdots i_n \in V_n^{G^c}, \\ 0 & \text{otherwise.} \end{cases} \tag{2.4}$$

It follows directly from the above definitions that

$$d_n = d_n^G + d_n^{G^c}. \tag{2.5}$$

Example 2.1. *Consider the complete graph K_3 with vertices $\{1, 2, 3\}$. Let G be the complete subgraph with vertices $\{1, 2\}$. Then*

$$\begin{aligned}
&V_0^G = \{1, 2\}, \quad V_1^G = \{12, 21\}, \quad V_2^G = \{121, 212\},\\
&V_0^{G^c} = \{3\}, \quad V_1^{G^c} = \{13, 23, 31, 32\},\\
&V_2^{G^c} = V_2^K \setminus V_2^G = \{123, 131, 132, 213, 231, 232, 312, 313, 321, 323\}.
\end{aligned}$$

$$d_0^G = \begin{bmatrix} -1 & 1 & 0\\ 1 & -1 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0 \end{bmatrix} \qquad \textit{and} \qquad d_0^{G^c} = \begin{bmatrix} 0 & 0 & 0\\ 0 & 0 & 0\\ -1 & 0 & 1\\ 0 & -1 & 1\\ 1 & 0 & -1\\ 0 & 1 & -1 \end{bmatrix}.$$

Notice that $d_0 = d_0^G + d_0^{G^c}$.

Let $\Delta_0 := (d_0^K)^* d_0^K$ be the Laplacian on 0-forms, where A^* denotes the transpose of A. For $n \geq 1$, let

$$\Delta_n^K := (d_n^K)^* d_n^K + d_{n-1}^K (d_{n-1}^K)^* \tag{2.6}$$

be the Laplacian on n-forms. Define Δ_n^G and $\Delta_n^{G^c}$ analogously.

Proposition 2.2. *The following relations hold.*

(a) *For any $n \geq 0$,*

$$(d_n^G)^*(d_n^{G^c}) = 0 \qquad \textit{and} \qquad (d_n^{G^c})^*(d_n^G) = 0. \tag{2.7}$$

(b) $\Delta_0^K = \Delta_0^G + \Delta_0^{G^c}$.

(c) *For any $n \geq 1$,*

$$\Delta_n^K = \Delta_n^G + \Delta_n^{G^c} + d_{n-1}^G (d_{n-1}^{G^c})^* + d_{n-1}^{G^c} (d_{n-1}^G)^*. \tag{2.8}$$

Proof. (a) Let $e^{i_0 \cdots i_n}$ be a canonical basis element of the vector space of all n-forms. Then by (2.3) and (2.4),

$$(d_n e^{i_0 \cdots i_n})_{j_0 \ldots j_{n+1}} = \begin{cases} (d_n^G e^{i_0 \cdots i_n})_{j_0 \ldots j_{n+1}}, & \text{if } j_0 \ldots j_{n+1} \in V_n^G,\\ (d_n^{G^c} e^{i_0 \cdots i_n})_{j_0 \ldots j_{n+1}}, & \text{if } j_0 \ldots j_{n+1} \in V_n^{G^c}. \end{cases} \tag{2.9}$$

Now by (2.1), the non-zero rows of $d_n^{G^c}$ are exactly the zero rows of d_n^G, i.e., the zero columns of $(d_n^G)^*$. Hence the equalities in 2.7 follow.

(b) By (2.5) and (2.7), we have

$$(d_n^K)^* d_n^K = (d_n^G + d_n^{G^c})^*(d_n^G + d_n^{G^c}) = (d_n^G)^* d_n^G + (d_n^{G^c})^* d_n^{G^c}. \tag{2.10}$$

Also, by using (2.5), we have

$$\begin{aligned}(d_{n-1}^K)(d_{n-1}^K)^* &= (d_{n-1}^G + d_{n-1}^{G^c})(d_{n-1}^G + d_{n-1}^{G^c})^* \\ &= d_{n-1}^G(d_{n-1}^G)^* + d_{n-1}^G(d_{n-1}^{G^c})^* + (d_{n-1}^{G^c})(d_{n-1}^G)^* + (d_{n-1}^{G^c})(d_{n-1}^{G^c})^*.\end{aligned} \tag{2.11}$$

Thus, (2.8) follows by combining (2.10), (2.11), and the definitions of $\Delta_n^K, \Delta_n^G, \Delta_n^{G^c}$. □

To simplify notation we let

$$L_{-1} := 0 \qquad \text{and} \qquad L_{n-1} := d_{n-1}^G(d_{n-1}^{G^c})^* + d_{n-1}^{G^c}(d_{n-1}^G)^* \quad \text{for } n \geq 1. \tag{2.12}$$

Proposition 2.3. *Let $n \geq 0$. Then for all $x, y \in V_n$ and $t \geq s \geq 0$,*

$$H_t^G(x,y) = H_t^K(x,y) - \int_0^t \Big(H_{t-s}^K(\Delta_n^{G^c} + L_{n-1})H_s^G\Big)(x,y)\, ds.$$

Proof. First, by the fundamental theorem of calculus,

$$\int_0^t \frac{\partial}{\partial s}\Big(\sum_{z\in V_n} H_s^G(z,y)H_{t-s}^K(x,z)\Big)\, ds = H_t^G(x,y) - H_t^K(x,y). \tag{2.13}$$

Computing the derivative on the left-side of (2.13), and using the symmetry of the operators $\Delta_n^G, \Delta_n^{G^c}$, and L_{n-1}, we get

$$\begin{aligned}
&\frac{\partial}{\partial s}\Big(\sum_{z\in V_n} H_s^G(z,y)H_{t-s}^K(x,z)\Big)\\
=&\sum_{z\in V_n}\Big(-H_{t-s}^K(x,z)\Delta_{n,z}^G H_s^G(z,y)+H_s^G(z,y)\Delta_{n,z}^K H_{t-s}^K(x,z)\Big)\\
=&\sum_{z\in V_n}\Big(-H_s^G(z,y)\Delta_{n,z}^G H_{t-s}^K(x,z)+H_s^G(z,y)\Delta_{n,z}^K H_{t-s}^K(x,z)\Big)\\
=&\sum_{z\in V_n} H_s^G(z,y)(\Delta_{n,z}^K-\Delta_{n,z}^G)H_{t-s}^K(x,z) \qquad (2.14)\\
=&\sum_{z\in V_n} H_s^G(z,y)(\Delta_{n,z}^{G^c}+L_{n-1,z})H_{t-s}^K(x,z) \qquad \text{(by (2.8) and (2.12))}\\
=&\sum_{z\in V_n} H_{t-s}^K(x,z)(\Delta_{n,z}^{G^c}+L_{n-1,z})H_s^G(z,y)\\
=&\Big(H_{t-s}^K(\Delta_n^{G^c}+L_{n-1})H_s^G\Big)(x,y).
\end{aligned}$$

Combining (2.13) and (2.14) yields the desired equality. □

Let $\mathcal{F}$ be the vector space of all real-valued functions on $[0,\infty)\times V_n^2$. Let $T:\mathcal{F}\to\mathcal{F}$ be a linear operator defined as

$$Tf_t(x,y) := -\int_0^t \Big(H_{t-s}^K(\Delta_n^{G^c}+L_{n-1})\Big)f_s(x,y)\,ds. \qquad (2.15)$$

Theorem 2.4. *Let T be defined as in* (2.15) *and assume that* $\|T\|<1$. *Then*

$$H_t^G(x,y)=\Big(\sum_{m=0}^{\infty}T^m\Big)H_t^K(x,y).$$

Proof. By Proposition 2.3,

$$\begin{aligned}
H_t^G(x,y)&=H_t^K(x,y)+TH_t^G(x,y)\\
&=H_t^K(x,y)+T\Big(H_t^K(x,y)+TH_t^G(x,y)\Big)\\
&=\cdots\\
&=(I+T+T^2+\cdots)H_t^K(x,y),
\end{aligned}$$

completing the proof. □

3. Heat kernel on 0-forms

A complete graph K_N has N vertices and $N(N-1)/2$ edges. The combinatorial Laplacian has eigenvalues 0 (with multiplicity 1) and N (with multiplicity $N-1$). Let V be the set of vertices of K_N. Let G be a sub-graph of K_N. Let G^c denote the complement of G obtained by removing those edges in K_N that appear in G.

Recall that the combinatorial Laplacian Δ on a graph is defined as $\Delta = A - D$, where A and D are the adjacency and degree matrices respectively. Let $H_t^K(x,y), H_t^G(x,y), H_t^{G^c}(x,y)$ denote the combinatorial Laplacians corresponding to K, G, G^c respectively. We use similar notation for the Laplacian Δ and the degree d_x of an element. Then

$$\Delta^K = \Delta^G + \Delta^{G^c}.$$

It is well known that that heat kernel associated to Δ^K is given by

$$H_t^K(x,y) = \begin{cases} \frac{1}{N} + (1-\frac{1}{N})e^{-Nt}, & x = y, \\ \frac{1}{N} - \frac{1}{N}e^{-Nt}, & x \neq y. \end{cases} \tag{3.1}$$

It can be obtained by expressing $H_t^K(x,y)$ in terms of the eigenfunctions and eigenvalues of Δ^K.

Proposition 3.1. *For all $x, y \in V$ and $t \geq 0$,*

$$H_t^G(x,y) = H_t^K(x,y) - e^{-Nt}\int_0^t e^{Ns}\Delta_x^{G^c} H_s^G(x,y)\, ds.$$

Proof. By using the proof of Proposition 2.3, we have

$$H_t^G(x,y) - H_t^K(x,y) = \int_0^t \sum_{z\in V} H_s^G(z,y)\Delta_z^{G^c} H_{t-s}^K(x,z)\, ds. \tag{3.2}$$

In view of (3.1), the integrand in (3.2) is equal to

$$\begin{aligned}
&\sum_{z\in V}\Big(\sum_{w\underset{G^c}{\sim}z}\Big[H^K_{t-s}(x,w)-H^K_{t-s}(x,z)\Big]\Big)H^G_s(z,y)\\
=&\Big(\sum_{w\underset{G^c}{\sim}x}\Big[H^K_{t-s}(x,w)-H^K_{t-s}(x,x)\Big]\Big)H^G_s(x,y)+\Big(\sum_{w\underset{G^c}{\sim}z,z\neq x}\Big[H^K_{t-s}(x,w)-H^K_{t-s}(x,z)\Big]\Big)H^G_s(z,y)\\
=&\sum_{w\underset{G^c}{\sim}x}-e^{-N(t-s)}H^G_s(x,y)+\sum_{w\underset{G^c}{\sim}z}\Big[H^K_{t-s}(x,x)-H^K_{t-s}(x,z)\Big]H^G_s(z,y)\\
=&\sum_{w\underset{G^c}{\sim}x}-e^{-N(t-s)}H^G_s(x,y)+\sum_{x\underset{G^c}{\sim}z}e^{-N(t-s)}H^G_s(z,y)\\
=&-e^{-N(t-s)}d^{G^c}_x H^G_s(x,y)+\sum_{x\underset{G^c}{\sim}z}e^{-N(t-s)}H^G_s(z,y)\\
=&-e^{-N(t-s)}\Big(d^{G^c}_x H^G_s(x,y)-\sum_{x\underset{G^c}{\sim}z}H^G_s(z,y)\Big)\\
=&-e^{-N(t-s)}\Delta^{G^c}_x H^G_s(x,y).
\end{aligned}$$

Substituting this into (3.2), we obtain the desired formula. □

Now let $\mathcal{F}$ be the space of all real-valued functions on $[0,\infty)\times V$. Let $T:\mathcal{F}\to\mathcal{F}$ be a linear operator defined as

$$Tu(t,x):=-e^{-Nt}\int_0^t e^{Ns}\Delta^{G^c}_x u(s,x)\,ds.$$

Let

$$\|u\|_\infty=\sup\Big\{|u(t,x)|:x\in V,t\in[0,\infty)\Big\}.$$

Proposition 3.2. *If $t<(1/N)\log(2(N-1)/(N-2))$, then $\|T\|<1$.*

Proof. It follows from definitions that

$$Tu(t,x)=-e^{-Nt}\int_0^t e^{Ns}\sum_{w\underset{G^c}{\sim}x}[u(s,w)-u(s,x)]\,ds.$$

Hence

$$\|Tu(t,x)\|\le e^{-Nt}\int_0^t e^{Ns}\cdot 2(N-1)\|u\|_\infty\,ds=\frac{2(N-1)}{N}(1-e^{-Nt})\|u\|_\infty.$$

Now, solving the inequality $2(N-1)(1-e^{-Nt})/N<1$ yields the stated upper bound for t below which one has $\|T\|<1$. □

Under the hypothesis of Proposition 3.2, $\|T\| < 1$ and thus by using Proposition 3.1,

$$H_t^G(x,y) = (I + T + T^2 + \cdots)H_t^K(x,y). \tag{3.3}$$

To derive a more explicit formula for $H_t^G(x,y)$, for each $y \in V$, we let $u_y : V \to V$ be the function defined as

$$u_y^{G^c}(x) := \begin{cases} d_x^{G^c} & \text{if } x = y, \\ 0 & \text{if } x \neq y \text{ and } x \underset{G}{\sim} y, \\ -1 & \text{if } x \neq y \text{ and } x \underset{G}{\not\sim} y. \end{cases} \tag{3.4}$$

Theorem 3.3. *Let $u_y^{G^c} : V \to V$ be defined as in* (3.4)*. Then for any $x, y \in V$, and all $t \geq 0$,*

$$\begin{aligned} H_t^G(x,y) &= H_t^K(x,y) + te^{-Nt}u_y^{G^c}(x) + e^{-Nt}\sum_{m=2}^{\infty}\frac{(-1)^{m-1}t^m}{m!}\left(\Delta_x^{G^c}\right)^{m-1}u_y^{G^c}(x) \\ &= \begin{cases} \frac{1}{N} - \frac{1}{N}e^{-Nt} + e^{-Nt}\sum_{m=1}^{\infty}\frac{(-1)^{m-1}t^m}{m!}\left(\Delta_x^{G^c}\right)^{m-1}u_y^{G^c}(x), & y \neq x, \\ \\ \frac{1}{N} + (1 - \frac{1}{N})e^{-Nt} + e^{-Nt}\sum_{m=1}^{\infty}\frac{(-1)^{m-1}t^m}{m!}\left(\Delta_x^{G^c}\right)^{m-1}u_y^{G^c}(x), & y = x, \end{cases} \end{aligned} \tag{3.5}$$

where $\left(\Delta_x^{G^c}\right)^{m-1}$ denotes the $(m-1)$-fold composition of $\Delta_x^{G^c}$ (or equivalently, the $(m-1)$th power of $\Delta_x^{G^c}$).

Proof. We first compute $TH_t^G(x,y)$ by considering the following three cases. Throughout the calculations below, we denote $x \underset{G^c}{\sim} y$ (i.e., x and y are neighbors in the graph G^c) simply by $x \sim y$.

Case 1. $x = y$. Then

$$\begin{aligned} TH_t^K(x,y) = TH_t^K(x,x) &= -e^{-Nt}\int_0^t e^{Ns}\Delta_x^{G^c}H_s^K(x,x)\,ds \\ &= -e^{-Nt}\int_0^t e^{Ns}\sum_{w\sim x}\left[H_s^K(w,x) - H_s^K(x,x)\right]ds \\ &= -e^{-Nt}\int_0^t e^{Ns}\sum_{w\sim x}(-e^{-Ns})\,ds \\ &= -e^{-Nt}\int_0^t e^{Ns}(-e^{-Ns})d_x^{G^c}\,ds \\ &= te^{-Nt}d_x^{G^c}. \end{aligned}$$

Case 2. $x \neq y$ and $x \sim y$. Then

$$\begin{aligned}
TH_t^K(x,y) &= -e^{-Nt}\int_0^t e^{Ns}\Delta_x^{G^c} H_s^K(x,y)\,ds \\
&= -e^{-Nt}\int_0^t e^{Ns}\sum_{w\sim x}\Big[H_s^K(w,y)-H_s^K(x,y)\Big]\,ds \\
&= -e^{-Nt}\int_0^t e^{Ns}\Big\{\sum_{w\sim x, w\neq y}\Big[H_s^K(w,y)-H_s^K(x,y)\Big]+\sum_{w\sim x, w=y}\Big[H_s^K(w,y)-H_s^K(x,y)\Big]\Big\}\,ds \\
&= -e^{-Nt}\int_0^t e^{Ns}(0+e^{-Ns})\,ds \\
&= -te^{-Nt}.
\end{aligned}$$

Case 3. $x \neq y$ and $x \not\sim y$. Then, unlike in Case 2, the situation $w \sim x$ and $w = y$ cannot occur. Hence

$$\begin{aligned}
TH_t^K(x,y) &= -e^{-Nt}\int_0^t e^{Ns}\Big(\sum_{w\sim x, w\neq y}\Big[H_s^K(w,y)-H_s^K(x,y)\Big]\Big)\,ds \\
&= -e^{-Nt}\int_0^t e^{Ns}\cdot 0\,ds \\
&= 0.
\end{aligned}$$

Thus,

$$TH_t^K(x,y) = te^{-Nt}u_y^{G^c}(x). \tag{3.6}$$

Now we can express $T^2H_t^K(x,y)$ conveniently as

$$\begin{aligned}
T^2H_t^K(x,y) &= -e^{-Nt}\int_0^t e^{Ns}\Delta_x^{G^c}\Big(TH_s^K(x,y)\Big)\,ds \\
&= -e^{-Nt}\int_0^t e^{Ns}\Delta_x^{G^c}\big(se^{-Ns}u_y^{G^c}(x)\big)\,ds \quad \text{(by (3.6))} \\
&= -e^{-Nt}\int_0^t s\Delta_x^{G^c}u_y^{G^c}(x)\,ds \\
&= -\frac{t^2e^{-Nt}}{2!}\Delta_x^{G^c}u_y^{G^c}(x).
\end{aligned}$$

By induction and a similar derivation, for all $m \geq 2$,

$$T^mH_t^K(x,y) = (-1)^{m-1}\frac{t^me^{-Nt}}{m!}\Big(\Delta_x^{G^c}\Big)^{m-1}u_y^{G^c}(x). \tag{3.7}$$

Combining this with equation (3.3) proves the proposition. □

By using (3.1), we can rewrite the formula for $H_t^G(x,y)$ in the following form.

Corollary 3.4. *The formula in Proposition 3.3 can be expressed as*

$$H_t^G(x,y) = \begin{cases} H_t^K(x,y)\Big(1 + \frac{N}{e^{Nt}+N-1}\sum_{m=1}^{\infty}\frac{(-1)^{m-1}t^m}{m!}(\Delta_x^{G^c})^{m-1}u_y^{G^c}(x)\Big), & y = x, \\ \\ H_t^K(x,y)\Big(1 + \frac{N}{e^{Nt}-1}\sum_{m=1}^{\infty}\frac{(-1)^{m-1}t^m}{m!}(\Delta_x^{G^c})^{m-1}u_y^{G^c}(x)\Big), & y \neq x. \end{cases}$$

We now study the radius of convergence of the power series in (3.5). We first prove a lemma.

Lemma 3.5. *For any $m \geq 1$ and any vertices $x, y \in V_0$,*

$$\left|(\Delta_x^{G^c})^{m-1}u_y^{G^c}(x)\right| \leq 2^{m-1}N^m.$$

Proof. The inequality clearly holds when $m = 1$. Assume that it holds for some $m \geq 1$. Then

$$\begin{aligned} \left|(\Delta_x G^c)^m u_y^{G^c}(x)\right| =& \left|\sum_{w \underset{G^c}{\sim} x}\Big[(\Delta_w^{G^c})^{m-1}u_y^{G^c}(w) - (\Delta_x)^{m-1}u_y^{G^c}(x)\Big]\right| \\ \leq& \sum_{w \underset{G^c}{\sim} x}\left(2^{m-1}N^m + 2^{m-1}N^m\right) \qquad \text{(Induction hypothesis)} \\ \leq& d_x^{G^c}2^mN^m \\ \leq& 2^mN^{m+1}, \end{aligned}$$

which completes the proof. ☐

Note that the series in Corollary 3.4 can also be written as

$$H_t^G(x,y) = \begin{cases} H_t^K(x,y)\Big(1 + \frac{Nt}{e^{Nt}+N-1}\sum_{m=1}^{\infty}\frac{(-1)^{m-1}t^{m-1}}{m!}(\Delta_x^{G^c})^{m-1}u_y^{G^c}(x)\Big), & y = x, \\ \\ H_t^K(x,y)\Big(1 + \frac{Nt}{e^{Nt}-1}\sum_{m=1}^{\infty}\frac{(-1)^{m-1}t^{m-1}}{m!}(\Delta_x^{G^c})^{m-1}u_y^{G^c}(x)\Big), & y \neq x. \end{cases} \tag{3.8}$$

Proposition 3.6. *Consider the expansion in Corollary 3.4.*

(a) *The radius of convergence of the series*

$$\sum_{m=1}^{\infty}\frac{(-1)^{m-1}t^m}{m!}\left(\Delta_x^{G^c}\right)^{m-1}u_y^{G^c}(x) \quad \text{and} \quad \sum_{m=1}^{\infty}\frac{(-1)^{m-1}t^m}{m!}\left(\Delta_x^{G^c}\right)^{m-1}u_y^{G^c}(x)$$

that appear in (3.5) *and* (3.8) *is* ∞.

(b) *The functions* $t/(e^{Nt}+N-1)$ *is real analytic in some open neighborhood of* 0, *and so is the function*

$$f(t) := \begin{cases} \dfrac{t}{e^{Nt}-1} & \text{if } t \neq 0, \\ \dfrac{1}{N} & \text{if } t = 0. \end{cases}$$

Proof. (a) By Stirling's formula, $m! \sim cm^{1/2+m}e^{-m}$ and hence $\sqrt[m]{m!} \sim Cm$ for some constant C. Thus, by Lemma 3.5, for all $x, y \in V_0$,

$$\begin{aligned} &\lim_{m\to\infty} \sqrt[m]{\left|\frac{(-1)^{m-1}t^m}{m!}(\Delta_x^{G^c})^{m-1}u_y^{G^c}(x)\right|} \\ \leq &\lim_{m\to\infty} \sqrt[m]{\left|\frac{|t|^m}{m!}2^m N^{m+1}\right|} \\ = &\lim_{m\to\infty} \frac{2N\sqrt[m]{N}|t|}{\sqrt[m]{m!}} \\ =&0. \end{aligned}$$

Hence the series converges for all $t \in \mathbb{R}$. The proof of the second series is the same.

(b) The function $t/(e^{Nt}+N-1)$ is clearly real analytic in some open neighborhood on 0. We now consider f. First, it is clear the f is continuous at 0. Let $f(z)$ be the extension of f to $\mathbb{C}$. Then

$$f(z) = \frac{1}{N\sum_{k=0}^{\infty}\frac{(Nz)^{k-1}}{k!}},$$

which is (complex) analytic on some open neighborhood of 0 in $\mathbb{C}$. Thus, $f(t)$ is real analytic on some open neighborhood of 0 in $\mathbb{R}$. □

Using Proposition 3.6 and Taylor series expansion, we can rewrite the heat kernel $H_t^G(x,y)$ in Corollary 3.4 in the following form.

Corollary 3.7. *Let* $u_y^{G^c}(x)$ *defined in* (3.4). *Then*

(a) *If* $y = x$, *then*

$$\begin{aligned} H_t^G(x,y) = H_t^K(x,y)\Bigg(&1 + d_x^{G^c}t - \frac{1}{2}\Big(2d_x^{G^c} + \Delta_x^{G^c}u_y^{G^c}(x)\Big)t^2 \\ &+ \frac{1}{6}\Big((6-3N)d_x^{G^c} + 3\Delta_x^{G^c}u_y^{G^c}(x) + (\Delta_x^{G^c})^2u_y^{G^c}(x)\Big)t^3 \\ &+ \frac{1}{12}\Big((-12+12N-2N^2)d_x^{G^c} - (6-3N)\Delta_x^{G^c}u_y^{G^c}(x) - (\Delta_x^{G^c})^2u_y^{G^c}(x)\Big)t^4 \\ &+ O(t^5)\Bigg). \end{aligned}$$

(b) *If* $y \neq x$ *and* $y \underset{G}{\sim} x$, *then*

$$H_t^G(x,y) = H_t^K(x,y)\Bigg(1 - \frac{1}{2}\Delta_x^{G^c} u_y^{G^c}(x)t + \frac{1}{12}\Big(3N\Delta_x^{G^c} u_y^{G^c}(x) + 2(\Delta_x^{G^c})^2 u_y^{G^c}(x)\Big)t^2 - \frac{1}{24}\Big(N^2\Delta_x^{G^c} u_y^{G^c}(x) + 2N(\Delta_x^{G^c})^2 u_y^{G^c}(x)\Big)t^3 + \frac{1}{72}N^2(\Delta_x^{G^c})^2 u_y^{G^c}(x)t^4 + O(t^5)\Bigg).$$

(c) *If* $y \neq x$ *and* $y \underset{G}{\not\sim} x$, *then*

$$H_t^G(x,y) = H_t^K(x,y)\Bigg(\frac{1}{2}\Big(N - \Delta_x^{G^c} u_y^{G^c}(x)\Big)t + \frac{1}{12}\Big(-N^2 + 3N\Delta_x^{G^c} u_y^{G^c}(x) + 2(\Delta_x^{G^c})^2 u_y^{G^c}(x)\Big)t^2 - \frac{1}{24}\Big(N^2\Delta_x^{G^c} u_y^{G^c}(x) + 2N(\Delta_x^{G^c})^2 u_y^{G^c}(x)\Big)t^3 + \frac{1}{720}\Big(N^4 + 10N^2(\Delta_x^{G^c})^2 u_y^{G^c}(x)\Big)t^4 + O\left(t^5\right)\Bigg).$$

4. Computing the coefficients in the heat kernel expansion

This section is devoted to the computation of the coefficients in the heat kernel expansion of $H_t^G(x,y)$. Let $c_k(x,y)$ be the coefficients of t^k in the above expression for $H_t^G(x,y)$. Then we see from the expression for $H_t^G(x,y)$ in Corollary 3.7 that

$$c_0(x,y) := \begin{cases} 1 & \text{if } x = y, \\ 1 & \text{if } x \neq y \text{ and } x \underset{G}{\sim} y, \\ 0 & \text{if } x \neq y \text{ and } x \underset{G}{\not\sim} y. \end{cases}$$

To compute the other coefficients, we let $\eta^{G,G}(x,y)$ be the number of G-neighbors of x that are also G-neighbors of y, and let $\eta^{G,G^c}(x,y)$ be the number of G-neighbors of x that are G^c-neighbors of y. Similarly we define $\eta^{G^c,G}(x,y)$ and $\eta^{G^c,G^c}(x,y)$. We first establish some elementary properties relating these quantities and d_x^G, $d_x^{G^c}$.

Since K is a complete graph, we have

$$d_x^G + d_x^{G^c} = N - 1. \tag{4.1}$$

The following elementary identities follow immediately from symmetry:

$$\begin{aligned} \eta^{G,G^c}(y,x) &= \eta^{G^c,G}(x,y), & \eta^{G,G}(y,x) &= \eta^{G,G}(x,y) \\ \eta^{G^c,G}(y,x) &= \eta^{G,G^c}(x,y), & \eta^{G^c,G^c}(y,x) &= \eta^{G^c,G^c}(x,y). \end{aligned} \tag{4.2}$$

Proposition 4.1. (a) *If $x \neq y$ and $x \underset{G}{\sim} y$, then*

$$d_x^G - 1 = \eta^{G,G}(x,y) + \eta^{G,G^c}(x,y), \tag{4.3}$$
$$d_x^{G^c} = \eta^{G^c,G}(x,y) + \eta^{G^c,G^c}(x,y). \tag{4.4}$$

(b) *If $x \neq y$ and $x \underset{G}{\not\sim} y$, then*

$$d_x^G = \eta^{G,G}(x,y) + \eta^{G,G^c}(x,y), \tag{4.5}$$
$$d_x^{G^c} - 1 = \eta^{G^c,G}(x,y) + \eta^{G^c,G^c}(x,y). \tag{4.6}$$

Proof. We only prove (b); the proof of (a) is similar. In this case, y is a G^c-neighbor of x. G-neighbors of x can be partitioned into two classes: those that are G-connected to y and those that are G^c-connected to y. This gives rise to (4.5).

As for (4.6), we note that y is G^c-neighbors of x. The remaining $d_c^{G^c} - 1$ G^c-neighbors of x can be partitioned into two classes: those that are G-connected to y and those that are G^c-connected to y. This proves (4.6). □

Proposition 4.2. (a) *If $x \neq y$ and $x \underset{G}{\sim} y$, then*

$$\begin{aligned} \eta^{G^c,G^c}(x,y) &= \eta^{G,G}(x,y) - d_x^G + d_y^{G^c} + 1 \\ &= \eta^{G,G}(x,y) + d_x^{G^c} - d_y^G + 1 \\ &= N + \eta^{G,G}(x,y) - d_x^G - d_y^G. \end{aligned} \tag{4.7}$$

(b) *If $x \neq y$ and $x \underset{G}{\not\sim} y$, then*

$$\begin{aligned} \eta^{G^c,G^c}(x,y) &= \eta^{G,G}(x,y) - d_x^G + d_y^{G^c} - 1 \\ &= \eta^{G,G}(x,y) + d_x^{G^c} - d_y^G - 1 \\ &= N - 2 - d_x^G - d_y^G + \eta^{G,G}(x,y). \end{aligned} \tag{4.8}$$

Proof. We will prove (a); the proof of (b) is similar. Interchanging the roles of x and y in (4.3) and using (4.2), we have

$$\begin{aligned} d_y^G - 1 &= \eta^{G,G}(y,x) + \eta^{G,G^c}(y,x) = \eta^{G,G}(x,y) + \eta^{G^c,G}(x,y), \\ d_y^{G^c} &= \eta^{G^c,G^c}(y,x) + \eta^{G^c,G}(y,x) = \eta^{G^c,G^c}(x,y) + \eta^{G,G^c}(x,y). \end{aligned} \tag{4.9}$$

Substituting these into (4.3) and (4.4) respectively, we get

$$\begin{aligned} d_x^G - 1 &= \eta^{G,G}(x,y) + d_y^{G^c} - \eta^{G^c,G^c}(x,y), \\ d_x^{G^c} &= \eta^{G^c,G^c}(x,y) + d_y^G - \eta^{G,G}(x,y) - 1, \end{aligned} \tag{4.10}$$

which imply the first two inequalities in (4.7), respectively. The third equality in (4.7) follows by using (4.2). □

Proposition 4.3.

$$\Delta_x^{G^c}\Big(u_y^{G^c}(x)\Big) = \begin{cases} -d_x^{G^c} - (d_x^{G^c})^2, & \text{if } x = y, \\ -\eta^{G^c,G^c}(x,y), & \text{if } x \neq y \text{ and } x \underset{G}{\sim} y, \\ -\eta^{G^c,G^c}(x,y) + d_x^{G^c} + d_y^{G^c}, & \text{if } x \neq y \text{ and } x \underset{G}{\not\sim} y, \end{cases}$$
$$= \begin{cases} -(N-1-d_x^G) - (N-1-d_x^G)^2, & \text{if } x = y, \\ -N - \eta^{G,G}(x,y) + d_x^G + d_y^G, & \text{if } x \neq y \text{ and } x \underset{G}{\sim} y, \\ N - \eta^{G,G}(x,y), & \text{if } x \neq y \text{ and } x \underset{G}{\not\sim} y. \end{cases}$$

Proof. Note that

$$\begin{aligned} \Delta_x^{G^c}\Big(u_y^{G^c}(x)\Big) &= (\Delta_x^K - \Delta_x^G)\Big(u_y^{G^c}(x)\Big) \\ &= \sum_{w \underset{K}{\sim} x} \Big(u_y^{G^c}(w) - u_y^{G^c}(x)\Big) - \sum_{w \underset{G}{\sim} x} \Big(u_y^{G^c}(w) - u_y^{G^c}(x)\Big) \\ &= \sum_{w \underset{G^c}{\sim} x} u_y^{G^c}(w) - \sum_{w \underset{G^c}{\sim} x} u_y^{G^c}(x). \end{aligned} \tag{4.11}$$

We divide the proof into three cases.

Case 1. $y = x$. In view of the definition of $u_y^{G^c}(x)$ and (4.11), we have

$$\begin{aligned} \Delta_x^{G^c}\Big(u_y^{G^c}(x)\Big) &= \sum_{w \underset{G^c}{\sim} x} (-1) - \sum_{w \underset{G^c}{\sim} x} d_x^{G^c} \\ &= -\, d_x^{G^c} - (d_x^{G^c})^2 \\ &= -\,(N-1-d_x^G) - (N-1-d_x^G)^2 \qquad \text{(by (4.1))}. \end{aligned}$$

Case 2. $y \neq x$ *and* $y \underset{G}{\sim} x$. Using (4.11) followed by Proposition 4.2(a), we have

$$\begin{aligned} \Delta_x^{G^c}\Big(u_y^{G^c}(x)\Big) &= \Bigg(\sum_{w \underset{G^c}{\sim} x, w \underset{G^c}{\sim} y} u_y^{G^c}(w) + \sum_{w \underset{G^c}{\sim} x, w \underset{G^c}{\not\sim} y} u_y^{G^c}(w)\Bigg) - d_x^{G^c} u_y^{G^c}(x) \\ &= \sum_{w \underset{G^c}{\sim} x, w \underset{G^c}{\sim} y} (-1) + 0 - 0 \\ &= -\eta^{G^c,G^c}(x,y) \\ &= -N - \eta^{G,G}(x,y) + d_x^G + d_y^G \qquad \text{(by Proposition 4.2(a))}. \end{aligned}$$

Case 3. $y \neq x$ *and* $y \underset{G}{\not\sim} x$. Using (4.11) followed by Proposition 4.2(b), we have

$$\begin{aligned}
\Delta_x^{G^c}\Big(u_y^{G^c}(x)\Big) &= \Big(\sum_{w \underset{G^c}{\sim} x, w \underset{G^c}{\sim} y} u_y^{G^c}(w) + \sum_{w \underset{G^c}{\sim} x, w \underset{G^c}{\not\sim} y} u_y^{G^c}(w)\Big) + u_y^{G^c}(y) - d_x^{G^c} u_y^{G^c}(x) \\
&= \sum_{w \underset{G^c}{\sim} x, w \underset{G^c}{\sim} y} (-1) + d_y^{G^c} + d_x^{G^c} \\
&= \eta^{G^c,G^c}(x,y) + d_y^{G^c} + d_x^{G^c} \\
&= N - \eta^{G,G}(x,y) \qquad \text{(by Proposition 4.2(b)).}
\end{aligned}$$

□

Proposition 4.4.

$$\begin{aligned}
&(\Delta_x^{G^c})^2\Big(u_y^{G^c}(x)\Big) \\
&= \begin{cases}
2(d_x^{G^c})^2 + (d_x^{G^c})^3 - \sum_{w \underset{G^c}{\sim} x} \eta^{G^c,G^c}(w,x) + \sum_{w \underset{G^c}{\sim} x} d_w^{G^c}, & x = y, \\[2ex]
(d_x^{G^c} + d_y^{G^c})\eta^{G^c,G^c}(x,y) - \sum_{w \underset{G^c}{\sim} x, w \neq y} \eta^{G^c,G^c}(w,y) \\
+ \sum_{w \underset{G^c}{\sim} x, w \neq y, w \underset{G^c}{\sim} y} d_w^{G^c}, & x \neq y \text{ and } x \underset{G}{\sim} y, \\[2ex]
-(d_x^{G^c})^2 - d_y^{G^c} - (d_y^{G^c})^2 - d_x^{G^c} d_y^{G^c} + (d_x^{G^c} + d_y^{G^c})\eta^{G^c,G^c}(x,y) \\
- \sum_{w \underset{G^c}{\sim} x, w \neq y} \eta^{G^c,G^c}(w,y) + \sum_{w \underset{G^c}{\sim} x, w \neq y, w \underset{G^c}{\sim} y} d_w^{G^c}, & x \neq y \text{ and } x \underset{G}{\not\sim} y,
\end{cases} \\[3ex]
&= \begin{cases}
-N^2 + N^3 - (1 - 3N + 3N^2) d_x^G - (2 - 3N)(d_x^G)^2 - (d_x^G)^3 \\
- \sum_{w \underset{G^c}{\sim} x} \eta^{G,G}(w,x), & x = y, \\[2ex]
-2 + 2N + 2N^2 - (1 + 3N) d_x^G + (d_x^G)^2 - 3N d_y^G + (d_y^G)^2 + d_x^G d_y^G \\
-(1 - 3N + d_x^G + d_y^G)\eta^{G,G}(x,y) \\
- \sum_{w \underset{G^c}{\sim} x, w \neq y, w \underset{G^c}{\sim} y} \eta^{G,G}(w,y) + \sum_{w \underset{G^c}{\sim} x, w \neq y, w \sim_G y} d_w^G, & x \neq y \text{ and } x \underset{G}{\sim} y, \\[2ex]
-N^2 + d_y^G - (3 - 3N + d_x^G + d_y^G)\eta^{G,G}(x,y) \\
- \sum_{w \underset{G^c}{\sim} x, w \neq y, w \underset{G^c}{\sim} y} \eta^{G,G}(w,y) + \sum_{w \underset{G^c}{\sim} x, w \neq y, w \sim_G y} (d_w^G - \eta^{G,G}(w,y)), & x \neq y \text{ and } x \underset{G}{\not\sim} y.
\end{cases}
\end{aligned}$$

Proof.

$$\begin{aligned}
(\Delta_x^{G^c})^2\Big(u_y^{G^c}(x)\Big) &= \sum_{w \underset{G^c}{\sim} x} \Big[\Delta_w^{G^c}\Big(u_y^{G^c}(w)\Big) - \Delta_x^{G^c}\Big(u_y^{G^c}(x)\Big)\Big] \\
&= \sum_{w \underset{G^c}{\sim} x} \Delta_w^{G^c}\Big(u_y^{G^c}(w)\Big) - d_x^{G^c} \Delta_x^{G^c}\Big(u_y^{G^c}(x)\Big).
\end{aligned} \tag{4.12}$$

We now apply the three cases of Proposition 4.3 to (4.12) as follows.

Case 1. $y = x$.

$$(\Delta_x^{G^c})^2\Big(u_y^{G^c}(x)\Big) = \sum_{w \underset{G^c}{\sim} x} \Big(-\eta^{G^c,G^c}(w,x) + d_x^{G^c} + d_w^{G^c}\Big) - d_x^{G^c}\Big(-d_x^{G^c} - (d_x^{G^c})^2\Big).$$

As $\sum_{w \underset{G^c}{\sim} x} d_x^{G^c} = (d_x^{G^c})^2$, the result follows.

Case 2. $y \neq x$ *and* $y \underset{G}{\sim} x$.

$$\begin{aligned}
(\Delta_x^{G^c})^2\Big(u_y^{G^c}(x)\Big) &= \sum_{w \underset{G^c}{\sim} x, w=y} \Delta_w^{G^c}\Big(u_y^{G^c}(w)\Big) + \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \Delta_w^{G^c}\Big(u_y^{G^c}(w)\Big)\\
&\quad + \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\not\sim} y} \Delta_w^{G^c}\Big(u_y^{G^c}(w)\Big) - d_x^{G^c}\Big(-\eta^{G^c,G^c}(x,y)\Big)\\
&= -d_y^{G^c} - (d_y^{G^c})^2 + \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \Big(-\eta^{G^c,G^c}(w,y) + d_y^{G^c} + d_w^{G^c}\Big)\\
&\quad - \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\not\sim} y} \eta^{G^c,G^c}(w,y) + d_x^{G^c}\eta^{G^c,G^c}(x,y)\\
&= -d_y^{G^c} - (d_y^{G^c})^2 - \sum_{w \underset{G^c}{\sim} x, w\neq y} \eta^{G^c,G^c}(w,y) + \eta^{G^c,G^c}(x,y) d_y^{G^c}\\
&\quad + \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} d_w^{G^c} + d_x^{G^c}\eta^{G^c,G^c}(x,y),
\end{aligned}$$

which equals the desired formula.

Case 3. $y \neq x$ *and* $y \underset{G}{\not\sim} x$.

$$
\begin{aligned}
(\Delta_x^{G^c})^2\Big(u_y^{G^c}(x)\Big) = &\sum_{w \underset{G^c}{\sim} x, w=y} \Delta_w^{G^c}\Big(u_y^{G^c}(w)\Big) + \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \Delta_w^{G^c}\Big(u_y^{G^c}(w)\Big) \\
&+ \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\not\sim} y} \Delta_w^{G^c}\Big(u_y^{G^c}(w)\Big) - d_x^{G^c}\Big(-\eta^{G^c,G^c}(x,y) + d_y^{G^c} + d_x^{G^c}\Big) \\
= &- d_y^{G^c} - (d_y^{G^c})^2 + \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \Big(-\eta^{G^c,G^c}(w,y) + d_y^{G^c} + d_w^{G^c}\Big) \\
&+ \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\not\sim} y} \Big(-\eta^{G^c,G^c}(w,y)\Big) - d_x^{G^c}\Big(-\eta^{G^c,G^c}(x,y) + d_y^{G^c} + d_x^{G^c}\Big) \\
= &- d_y^{G^c} - (d_y^{G^c})^2 - \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \Big(-\eta^{G^c,G^c}(w,y) - d_w^{G^c}\Big) + \eta^{G^c,G^c}(x,y) d_y^{G^c} \\
&- \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\not\sim} y} \eta^{G^c,G^c}(w,y) + d_x^{G^c}\eta^{G^c,G^c}(x,y) - d_x^{G^c} d_y^{G^c} - \Big(d_x^{G^c}\Big)^2,
\end{aligned}
$$

and the desired formula follows. □

From the expansion of $H_t^G(x,y)$, we have

$$
c_1(x,y) = \begin{cases} d_x^{G^c}, & \text{if } x = y, \\ -\frac{1}{2}\Delta_x^{G^c} u_y^{G^c}(x), & \text{if } x \neq y \text{ and } x \underset{G}{\sim} y, \\ \frac{1}{2}\Big(N - \Delta_x^{G^c} u_y^{G^c}(x)\Big), & \text{if } x \neq y \text{ and } x \underset{G}{\not\sim} y. \end{cases} \tag{4.13}
$$

By using Proposition 4.3, we obtain the following expression for $c_1(x,y)$ involving G and not G^c, which also shows the equality of $a_1(x,y)$ and $c_1(x,y)$. For all $x, y \in K$, we can verify directly that

$$
a_1(x,y) = c_1(x,y).
$$

In fact, using Proposition 4.3 and (4.13), followed by Proposition 4.2 and (4.1), we get

Proposition 4.5.

$$
\begin{aligned}
c_1(x,y) &= \begin{cases} d_x^{G^c} & \textit{if } x = y, \\ \frac{1}{2}\eta^{G^c,G^c}(x,y) & \textit{if } x \neq y \textit{ and } x \underset{G}{\sim} y, \\ \frac{1}{2}\Big(N - d_x^{G^c} - d_y^{G^c} + \eta^{G^c,G^c}(x,y)\Big) & \textit{if } x \neq y \textit{ and } x \underset{G}{\not\sim} y, \end{cases} \\
&= \begin{cases} N - 1 - d_x^{G} & \textit{if } x = y, \\ \frac{1}{2}\Big(N + \eta^{G,G}(x,y) - d_x^{G} - d_y^{G}\Big) & \textit{if } x \neq y \textit{ and } x \underset{G}{\sim} y, \\ \frac{1}{2}\eta^{G,G}(x,y) & \textit{if } x \neq y \textit{ and } x \underset{G}{\not\sim} y. \end{cases}
\end{aligned}
$$

Proposition 4.6. (a) *If $x = y$, then*

$$c_2(x,y) = \frac{1}{2}\Big(N^2 - 3N + 2 + (3-2N)d_x^G + (d_x^G)^2\Big).$$

(b) *If $x \neq y$ and $x \underset{G}{\sim} y$, then*

$$\begin{aligned}c_2(x,y) = \frac{1}{12}\Bigg(& -4 + 4N + N^2 - (2+3N)d_x^G - 3Nd_y^G + 2(d_y^G)^2 + 2d_x^G d_y^G \\ & - \big(2 - 3N + 2d_x^G + 2d_y^G\big)\eta^{G,G}(x,y) \\ & - 2 \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \eta^{G,G}(w,y) + 2 \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G}{\sim} y} d_w^G \Bigg).\end{aligned}$$

(c) *If $x \neq y$ and $x \underset{G}{\not\sim} y$, then*

$$\begin{aligned}c_2(x,y) = \frac{1}{12}\Bigg(& 2d_y^G - \big(9 - 6N + 2d_x^G + 2d_y^G\big)\eta^{G,G}(x,y) \\ & - 2 \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \eta^{G,G}(w,y) + 2 \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G}{\sim} y} (d_w^G - \eta^{G,G}(w,y)) \Bigg).\end{aligned}$$

Proof. (a) Using the expansion formula for $H_t^G(x,y)$, we have

$$\begin{aligned}c_2(x,y) &= -d_x^{G^c} - \frac{1}{2}\Delta_x^{G^c} u_y^{G^c}(x) \\ &= -d_x^{G^c} - \frac{1}{2}(-d_x^{G^c} - (d_x^{G^c})^2) \\ &= -\frac{1}{2}d_x^{G^c} + \frac{1}{2}(d_x^{G^c})^2 \\ &= -\frac{1}{2}(N - 1 - d_x^G) + \frac{1}{2}(N-1-d_x^G)^2 \\ &= \frac{1}{2}\Big(N^2 - 3N + 2 + (3-2N)d_x^G + (d_x^G)^2\Big),\end{aligned}$$

which is equal to $a_2(x,x)$.

We will prove part (b); the proof of (c) is similar. According to the expression for $H_t^G(x,y)$ at the beginning of this section,

$$c_2(x,y) = \frac{1}{4}N\Delta_x^{G^c}\Big(u_y^{G^c}(x)\Big) + \frac{1}{6}(\Delta_x^{G^c})^2\Big(u_y^{G^c}(x)\Big).$$

By using Propositions 4.3 and 4.4, we get

$$
\begin{aligned}
c_2(x,y) =& \frac{1}{4}N\Big(-N + d_x^G + d_y^G - \eta^{G,G}(x,y)\Big) \\
&+ \frac{1}{6}\Bigg(-2 + 2N + 2N^2 - (1-3N)d_x^G + (d_x^G)^2 - 3Nd_y^G + (d_y^G)^2 + d_x^G d_y^G \\
&\qquad - (1 - 3N + d_x^G + d_y^G)\eta^{G,G}(x,y) \\
&\qquad - \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \eta^{G,G}(w,y) + \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G}{\sim} y} d_w^G \Bigg),
\end{aligned}
$$

which can be simplified to the stated formula.

The coefficients of $c_3(x,y)$ can be obtained as in Proposition 4.6. We state the result below and omit the proof.

Proposition 4.7. *The coefficients $c_3(x,y)$ are as follows.*

(a) *If $x = y$,*

$$
\begin{aligned}
c_3(x,y) = -\frac{1}{6}\Bigg(& 6 - 12N + 7N^2 - N^3 + (10 - 12N + 3N^2)d_x^G + (5-3N)(d_x^G)^2 + (d_x^G)^3 \\
& - \sum_{w \underset{G^c}{\sim} x} \eta^{G,G}(w,x)\Bigg).
\end{aligned}
$$

(b) *If $x \neq y$ and $x \underset{G}{\sim} y$, then*

$$
\begin{aligned}
c_3(x,y) = -\frac{1}{24}\Bigg(& -4N + 4N^2 + 5N^3 - (2N + 7N^2)d_x^G + 2N(d_x^G)^2 + 2Nd_x^G d_y^G \\
& - 7N^2 d_y^G + 2N(d_y^G)^2 + (-2N + 2Nd_x^G - 2Nd_y^G)\eta^{G,G}(x,y) \\
& - 2N \sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \eta^{G,G}(w,y) + 2N \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G}{\sim} y} d_w^G \Bigg)
\end{aligned}
$$

(c) *If $x \neq y$ and $x \underset{G}{\not\sim} y$, then*

$$
\begin{aligned}
c_3(x,y) = -\frac{1}{24}\Bigg(& -N^3 + 2Nd_y^G - \big(6N - 5N^2 + 2d_x^G + 2d_y^G\big)\eta^{G,G}(x,y) \\
& - 2N \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G^c}{\sim} y} \eta^{G,G}(w,y) + 2N \sum_{w \underset{G^c}{\sim} x, w\neq y, w \underset{G}{\sim} y} (d_w^G - \eta^{G,G}(w,y))\Bigg).
\end{aligned}
$$

□

5. A second method for finding heat kernel expansion

In this section, we use a second method to obtain the heat kernel expansion. The method is analogous to one on Riemannian manifolds (see [1, 12, 13]). The coefficients of the expansion for $H_t^G(x,y)$ obtained by using the two methods appear in quite different forms. The fact that they must equal give us identities relating various quantities that appear in the expansions. We can verify that the first few of these coefficients are indeed the same by converting one to another.

First, we may expand the heat kernel on K in (3.1) as follows:

$$\begin{aligned} &H_t^K(x,y)\\ &=\begin{cases} 1-(N-1)t+\frac{1}{2}N(N-1)t^2-\frac{1}{6}N^2(N-1)t^3+\frac{1}{24}N^3(N-1)t^4+O\left(t^5\right), & x=y,\\ t-\frac{1}{2}Nt^2+\frac{1}{6}N^2t^3-\frac{1}{24}N^3t^4+O(t^5), & x\neq y. \end{cases} \end{aligned} \tag{5.1}$$

Here and throughout this paper, an asymptotic order of the form $O(t^k)$, $k>0$, holds as $t\to 0^+$.

Next, using Proposition 3.6, we can write

$$H_t^G(x,y) := H_t^K(x,y)\Big(a_0(x,y)+a_1(x,y)t+a_2(x,y)t^2+a_3(x,y)t^3+\cdots\Big).$$

We remark that this method is not completely independent of the previous one, which guarantees that such an expansion is valid on some open interval containing 0.

Now, in view of (5.1), if $x=y$, then

$$\begin{aligned} H_t^G(x,x) &= a_0(x,x)+\Big(-(N-1)a_0(x,x)+a_1(x,x)\Big)t\\ &\quad+\left(\frac{1}{2}N(N-1)a_0(x,x)-(N-1)a_1(x,x)+a_2(x,x)\right)t^2\\ &\quad+\left(-\frac{1}{6}N^2(N-1)a_0(x,x)+\frac{1}{2}N(N-1)a_1(x,x)-(N-1)a_2(x,x)+a_3(x,x)\right)t^3\\ &\quad+\left(\frac{1}{24}N^3(N-1)a_0(x,y)-\frac{1}{6}N^2(N-1)a_1(x,y)\right.\\ &\qquad\left.+\frac{1}{2}N(N-1)a_2(x,y)-(N-1)a_3(x,y)+a_4(x,y)\right)t^4\\ &\quad+O\left(t^5\right). \end{aligned} \tag{5.2}$$

If $x\neq y$, then

$$\begin{aligned} H_t^G(x,y) &= a_0(x,y)t+\left(-\frac{1}{2}Na_0(x,y)+a_1(x,y)\right)t^2\\ &\quad+\left(\frac{1}{6}N^2a_0(x,y)-\frac{1}{2}Na_1(x,y)+a_2(x,y)\right)t^3\\ &\quad+\left(-\frac{1}{24}N^3a_0(x,y)+\frac{1}{6}N^2a_1(x,y)-\frac{1}{2}Na_2(x,y)+a_3(x,y)\right)t^4+O(t^5), \end{aligned} \tag{5.3}$$

By using (5.2) and (5.3), we obtain the following partial derivatives with respect to t. If $x = y$, then

$$\begin{aligned}\frac{\partial H_t^G(x,x)}{\partial t} &= -(N-1)a_0(x,x) + a_1(x,x) \\ &+ \Big(N(N-1)a_0(x,x) - 2(N-1)a_1(x,x) + 2a_2(x,x)\Big)t \\ &+ \left(-\frac{1}{2}N^2(N-1)a_0(x,x) + \frac{3}{2}N(N-1)a_1(x,x) - 3(N-1)a_2(x,x) + 3a_3(x,x)\right)t^2 \\ &+ \bigg(\frac{1}{6}N^3(N-1)a_0(x,y) - \frac{2}{3}N^2(N-1)a_1(x,y) \\ &\quad + 2N(N-1)a_2(x,y) - 4(N-1)a_3(x,y) + 4a_4(x,y)\bigg)t^3 + O\left(t^4\right).\end{aligned} \tag{5.4}$$

If $x \neq y$,

$$\begin{aligned}\frac{\partial H_t^G(x,y)}{\partial t} &= a_0(x,y) + \Big(-Na_0(x,y) + 2a_1(x,y)\Big)t \\ &+ \left(\frac{1}{2}N^2a_0(x,y) - \frac{3}{2}Na_1(x,y) + 3a_2(x,y)\right)t^2 \\ &+ \left(-\frac{1}{6}N^3a_0(x,y) + \frac{2}{3}N^2a_1(x,y) - 2Na_2(x,y) + 4a_3(x,y)\right)t^3 \\ &+ O\left(t^4\right).\end{aligned} \tag{5.5}$$

We now compute the Laplacian Δ_x^G of $H_t^G(x,y)$. If $x = y$, then

$$\begin{aligned}\Delta_x^G H_t^G(x,x) &= -d_x^G a_0(x,x) + \Big[-d_x^G\Big(-(N-1)a_0(x,x) + a_1(x,x)\Big) + \sum_{w \underset{G}{\sim} x} a_0(w,x)\Big]t \\ &+ \Big[\sum_{w \underset{G}{\sim} x}\Big(a_1(w,x) - \frac{1}{2}Na_0(w,x)\Big) - d_x^G\Big(\frac{1}{2}N(N-1)a_0(x,x) - (N-1)a_1(x,x) + a_2(x,x)\Big)\Big]t^2 \\ &+ \Big[\sum_{w \underset{G}{\sim} x}\Big(\frac{1}{6}N^2a_0(w,x) - \frac{1}{2}Na_1(w,x) + a_2(w,x)\Big) - d_x^G\Big(-\frac{1}{6}N^2(N-1)a_0(x,x) \\ &\quad + \frac{1}{2}N(N-1)a_1(x,x) - (N-1)a_2(x,x) + a_3(x,x)\Big)\Big]t^3 \\ &+ \Big[\sum_{w \underset{G}{\sim} x}\Big(-\frac{1}{24}N^3a_0(w,x) + \frac{1}{6}N^2a_1(w,x) - \frac{1}{2}Na_2(w,x) + a_3(w,x)\Big) \\ &\quad - d_x^G\Big(\frac{1}{24}N^3(N-1)a_0(x,x) - \frac{1}{6}N^2(N-1)a_1(x,x) + \frac{1}{2}N(N-1)a_2(x,x) \\ &\quad - (N-1)a_3(x,x) + a_4(x,x)\Big)\Big]t^4 + O\left(t^5\right)\end{aligned} \tag{5.6}$$

If $x \neq y$, we have

$$\begin{aligned}\Delta_x^G H_t^G(x,y) = a_0(y,y) + \Big[&- d_x^G a_0(x,y) - (N-1)a_0(y,y) + a_1(y,y) + \sum_{w \underset{G}{\sim} x, w\neq y} a_0(w,y)\Big] t \\
+ \Big[- d_x^G \Big(a_1(x,y) &- \frac{1}{2} N a_0(x,y)\Big) + \sum_{w \underset{G}{\sim} x, w\neq y} \Big(a_1(w,y) - \frac{1}{2} N a_0(w,y)\Big) \\
&+ \frac{1}{2} N(N-1) a_0(y,y) - (N-1)a_1(y,y) + a_2(y,y)\Big] t^2 \\
+ \Big[- d_x^G \Big(\frac{1}{6} N^2 &a_0(x,y) - \frac{1}{2} N a_1(x,y) + a_2(x,y)\Big) \\
&+ \sum_{w \underset{G}{\sim} x, w\neq y} \Big(\frac{1}{6} N^2 a_0(w,y) - \frac{1}{2} N a_1(w,y) + a_2(w,y)\Big) \\
&- \frac{1}{6} N^2(N-1) a_0(y,y) + \frac{1}{2} N(N-1) a_1(y,y) \\
&- (N-1) a_2(y,y) + a_3(y,y)\Big] t^3 \\
+ \Big[- d_x^G \Big(- \frac{1}{24} &N^3 a_0(x,y) + \frac{1}{6} N^2 a_1(x,y) - \frac{1}{2} N a_2(x,y) + a_3(x,y)\Big) \\
&+ \sum_{w \underset{G}{\sim} x, w\neq y} \Big(- \frac{1}{24} N^3 a_0(w,y) + \frac{1}{6} N^2 a_1(w,y) - \frac{1}{2} N a_2(w,y) + a_3(w,y)\Big) \\
&+ \frac{1}{24} N^3(N-1) a_0(y,y) - \frac{1}{6} N^2(N-1) a_1(y,y) \\
&+ \frac{1}{2} N(N-1) a_2(y,y) - (N-1) a_3(y,y) + a_4(y,y)\Big] t^4 + O\left(t^5\right).\end{aligned} \tag{5.7}$$

To compute the coefficients $a_i(x,y)$, we let $\eta^G(x,y)$ be the number of G-neighbors of x that are also G-neighbors of y.

Proposition 5.1. *The coefficients $a_i(x,y)$, $i = 0,1,2,3$ are as follows:*

(a)

$$\begin{aligned} a_0(x,y) &= \begin{cases} 1 & \text{if } x = y, \\ 1 & \text{if } x \neq y \text{ and } x \underset{G}{\sim} y, \\ 0 & \text{if } x \neq y \text{ and } x \underset{G}{\not\sim} y, \end{cases} \\ &= c_0(x,y). \end{aligned}$$

(b)

$$\begin{aligned} a_1(x,y) &= \begin{cases} N - 1 - d_x^G & \text{if } x = y, \\ \frac{1}{2}\Big(N - d_x^G - d_y^G + \eta^G(x,y)\Big) & \text{if } x \neq y \text{ and } x \underset{G}{\sim} y, \\ \frac{1}{2} \eta^G(x,y) & \text{if } x \neq y \text{ and } x \underset{G}{\not\sim} y. \end{cases} \\ &= c_1(x,y) \end{aligned}$$

(c)

$$a_2(x,y) = \begin{cases} \frac{1}{2}\Big(N^2 - 3N + 2 + (3-2N)d_x^G + (d_x^G)^2\Big), & \textit{if } x = y, \\ \frac{1}{12}\Big(N^2 - 3Nd_x^G + 2(d_x^G)^2 + (2-3N)d_y^G + 2(d_y^G)^2 + 2d_x^G d_y^G \\ \quad + (3N - 2d_x^G - 2d_y^G)\eta^G(x,y) \\ \quad - 2\sum\limits_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} d_w^G + 2\sum\limits_{w \underset{G}{\sim} x, w \neq y} \eta^G(w,y)\Big), & \textit{if } x \neq y \textit{ and } x \underset{G}{\sim} y, \\ \frac{1}{12}\Big((3N - 2d_x^G - 2d_y^G)\eta^G(x,y) \\ \quad - 2\sum\limits_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} d_w^G + 2\sum\limits_{w \underset{G}{\sim} x, w \neq y} \eta^G(w,y)\Big), & \textit{if } x \neq y \textit{ and } x \underset{G}{\not\sim} y. \end{cases}$$

In particular, this verifies that $a_2(x,x) = c_2(x,x)$.

Proof. To find $a_i(x,y)$, we set

$$\Delta_x^G H_t^G(x,y) = \frac{\partial H_t^G(x,y)}{\partial t} \tag{5.8}$$

and equate the coefficients of t^i for $i \in \mathbb{N}$.

(a) When $t = 0$, $H_0(x,y) = \delta_{x,y}$. We impose the same condition on $H_t^G(x,y)$.

Case 1. $x = y$. Substituting $t = 0$ in (5.2) gives

$$a_0(x,x) = 1 \quad \text{for all } x. \tag{5.9}$$

To find $a_0(x,y)$ for $x \neq y$, consider the following two cases:

Case 2. $x \neq y$ *and* $x \underset{G}{\sim} y$. By using (5.8), (5.5), and (5.7), we have

$$a_0(x,y) = a_0(y,y) = 1.$$

In view of (5.9) and (5.3), we have

$$a_0(x,y) = a_0(y,y) = 1 \quad \text{for all } x. \tag{5.10}$$

Case 3. $x \neq y$ *and* $x \underset{G}{\not\sim} y$. By using (5.9), (5.3), and (5.7), we get

$$a_0(x,y) = 0.$$

This proves (a).

(b) Again we divide the the three cases separately.

Case 1. $x = y$. Equating the constant terms of (5.4) and (5.6), we have

$$(1-N)a_0(x,x) + a_1(x,x) = -d_x^G a_0(x,x).$$

Thus,

$$a_1(x,x) = N - 1 - d_x^G. \tag{5.11}$$

Case 2. $x \neq y$ *and* $x \underset{G}{\sim} y$. Equating the coefficients of t in (5.5) and (5.7), and then using part (a) and (5.11), we have

$$-Na_0(x,y) + 2a_1(x,y) = (1-N)a_0(y,y) + a_1(y,y) - d_x^G a_0(x,y) + \sum_{w \underset{G}{\sim} x, w \neq y} a_0(w,y),$$

which gives

$$a_1(x,y) = \frac{1}{2}\Big(N - d_x^G - d_y^G + \sum_{w \underset{G}{\sim} x, x \neq y} a_0(w,y)\Big).$$

But

$$\begin{aligned}\sum_{w \underset{G}{\sim} x, w \neq y} a_0(w,y) &= \sum_{w \underset{G}{\sim} x, w \neq y, y \sim x} a_0(w,y) + \sum_{w \underset{G}{\sim} x, w \neq y, y \underset{G}{\not\sim} w} a_0(w,y) \\ &= \sum_{w \underset{G}{\sim} x, w \neq y, y \underset{G}{\sim} w} 1 + \sum_{w \underset{G}{\sim} x, w \neq y, y \underset{G}{\not\sim} w} 0 \\ &= \eta^G(x,y),\end{aligned}$$

which proves the asserted expression for $a_1(x,y)$.

Case 3. $x \neq y$ *and* $x \underset{G}{\not\sim} y$. Equating the coefficients of t in (5.5) and (5.7), and then using part (a) and (5.11), we have

$$-Na_0(x,y) + 2a_1(x,y) = -d_x^G a_0(x,y) + \sum_{w \underset{G}{\sim} y, w \neq y} a_0(w,y),$$

which implies that

$$
\begin{aligned}
a_1(x,y) &= \frac{1}{2} \sum_{w \underset{G}{\sim} x, w \neq y} a_0(x,y) \\
&= \frac{1}{2}\Big(\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} + \sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} a_0(w,y)\Big) \\
&= \frac{1}{2}\eta^G(x,y).
\end{aligned}
$$

(c) $a_2(x,y)$ can be found similarly.

Case 1. $y = x$. Equating the coefficients of t in (5.4) and (5.6), we have

$$
N(N-1)a_0(x,x) + 2(1-N)a_1(x,x) + 2a_2(x,x) = -d_x^G\Big((1-N)a_0(x,x) + a_1(x,x)\Big) + \sum_{w \underset{G}{\sim} x} a_0(w,x).
$$

Substituting $a_0(x,x) = 1$, $a_0(w,x) = 1$ if $w \underset{G}{\sim} x$, and $a_1(x,x) = N - 1 - d_x^G$ gives

$$
a_2(x,x) = \frac{1}{2}\Big((d_x^G)^2 + (3-2N)d_x^G + N^2 - 3N + 2\Big). \tag{5.12}
$$

Case 2. $y \neq x$ and $y \underset{G}{\sim} x$. Again, equating the coefficients of t^2 in (5.5) and (5.7) gives

$$
a_2(x,y) = \frac{1}{12}\Bigg(3N\eta^G(x,y) - 2d_x^G\eta^G(x,y) + 4\sum_{w \underset{G}{\sim} x, w\neq y}\Big(a_1(w,y) - \frac{1}{2}Na_0(w,y)\Big)\Bigg). \tag{5.13}
$$

The desired formula now follows by using the expression in (5.15).

Case 3. $y \neq x$ and $y \underset{G}{\not\sim} x$. We equate the coefficients of t^2 in (5.5) and (5.7) to get

$$
\begin{aligned}
&\frac{1}{2}N^2 a_0(x,y) - \frac{3}{2}Na_1(x,y) + 3a_2(x,y) \\
=& - d_x^G\Big(a_1(x,y) - \frac{1}{2}Na_0(x,y)\Big) + \sum_{w \underset{G}{\sim} x, w\neq y}\Big(a_1(w,y) - \frac{1}{2}Na_0(w,y)\Big) \\
&+ \frac{1}{2}N(N-1)a_0(y,y) + (1-N)a_1(y,y) + a_2(y,y).
\end{aligned} \tag{5.14}
$$

The second term on the right-hand side can be simplified as

$$\begin{aligned}
&\sum_{w \underset{G}{\sim} x, w\neq y} \Big(a_1(w,y) - \frac{1}{2}Na_0(w,y)\Big) \\
=&\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} \Big(-\frac{1}{2}Na_0(w,y) + a_1(w,y)\Big) + \sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\not\sim} y} \Big(-\frac{1}{2}Na_0(w,y) + a_1(w,y)\Big) \\
=&\frac{1}{2}\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} \Big(-d_w^G - d_y^G + \eta^G(w,y)\Big) + \frac{1}{2}\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\not\sim} y} \eta^G(w,y) \\
=&-\frac{1}{2}\eta^G(x,y)d_y^G + \frac{1}{2}\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} \Big(-d_w^G + \eta^G(w,y)\Big) + \frac{1}{2}\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\not\sim} y} \eta^G(w,y) \\
=&-\frac{1}{2}\eta^G(x,y)d_y^G - \frac{1}{2}\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} d_w^G + \frac{1}{2}\Big(\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} + \sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\not\sim} y}\Big)\eta^G(w,y) \\
=&-\frac{1}{2}\eta^G(x,y)d_y^G - \frac{1}{2}\sum_{w \underset{G}{\sim} x, w\neq y, w \underset{G}{\sim} y} d_w^G + \frac{1}{2}\sum_{w \underset{G}{\sim} x, w\neq y} \eta^G(w,y).
\end{aligned} \tag{5.15}$$

Substituting this and the known values of a_0 and a_1 into (5.14) we get the desired expression for $a_2(x,y)$. We remark that $a_k(x,y)$, $k \geq 3$ can be computed by using the same method but the formulas get increasingly complicated.

□

6. Heat kernel of Laplacian on 1-forms on subgraphs of a complete graph

Let $K = K_N$ be the complete graph with N vertext set $V_0 := \{1, 2, \ldots, N\}$. Let $V_1 := \{ij : i, j \in V_0, i \neq j\}$ denote the set of directed edges

There are six heat kernels for the Laplacian on 1-forms on K_N:

$$\begin{aligned}
&u_1(t) := H_t^K(w_{ij}, w_{ij}), \qquad u_2(t) := H_t^K(w_{ij}, w_{ji}), \qquad u_3(t) := H_t^K(w_{ij}, w_{jk}), \\
&u_4(t) := H_t^K(w_{ij}, w_{kj}), \qquad u_5(t) := H_t^K(w_{ij}, w_{ik}), \qquad u_6(t) := H_t^K(w_{ij}, w_{kl}),
\end{aligned}$$

where i, j, k, l are distinct indices. The heat kernels satisfy the following heat equation for 1-forms (see, e.g., [3]):

$$\frac{\partial}{\partial t}H_t(\omega_{ij}, \cdot) = \Delta H_t(\omega_{ij}, \cdot),$$

where

$$\Delta H_t(\omega_{ij}, \cdot) = -(3N-2)H_t(\omega_{ij}, \cdot) + \sum_{\alpha\neq i,j} \big[H_t(\omega_{\alpha j}, \cdot) + H_t(\omega_{i\alpha}, \cdot)\big].$$

We obtain the following six ODEs with initial values

$$H_0(\omega_{ij},\omega_{kl}) = \begin{cases} 1 & \text{if } \omega_{kl}=\omega_{ij}, \\ 0 & \text{otherwise.} \end{cases}$$

$$\begin{aligned}(1)\quad \frac{\partial}{\partial t}H_t(\omega_{ij},\omega_{ij}) =&\Delta H_t(\omega_{ij},\omega_{ij}) \\ =&-(3N-2)H_t(\omega_{ij},\omega_{ij})+\sum_{\alpha\neq i,j}[H_t(\omega_{\alpha j},\omega_{ij})+H_t(\omega_{i\alpha},\omega_{ij})] \\ =&-(3N-2)H_t(\omega_{ij},\omega_{ij})+(N-2)H_t(\omega_{\alpha j},\omega_{ij})+(N-2)H_t(\omega_{i\alpha},\omega_{ij}) \\ =&-(3N-2)u_1+(N-2)u_4+(N-2)u_5.\end{aligned}$$

$$\begin{aligned}(2)\quad \frac{\partial}{\partial t}H_t(\omega_{ij},\omega_{ji}) =&\Delta H_t(\omega_{ij},\omega_{ji}) \\ =&-(3N-2)H_t(\omega_{ij},\omega_{ji})+\sum_{\alpha\neq i,j}[H_t(\omega_{\alpha j},\omega_{ji})+H_t(\omega_{i\alpha},\omega_{ji})] \\ =&-(3N-2)H_t(\omega_{ij},\omega_{ji})+(N-2)H_t(\omega_{\alpha j},\omega_{ji})+(N-2)H_t(\omega_{ji},\omega_{i\alpha}) \\ =&-(3N-2)u_2+2(N-2)u_3.\end{aligned}$$

$$\begin{aligned}(3)\quad \frac{\partial}{\partial t}H_t(\omega_{ij},\omega_{jk}) =&\Delta H_t(\omega_{ij},\omega_{jk}) \\ =&-(3N-2)H_t(\omega_{ij},\omega_{jk})+\sum_{\alpha\neq i,j}[H_t(\omega_{\alpha j},\omega_{jk})+H_t(\omega_{i\alpha},\omega_{jk})] \\ =&-(3N-2)H_t(\omega_{ij},\omega_{jk})+H_t(\omega_{kj},\omega_{jk})+(N-3)u_3+H_t(\omega_{ik},\omega_{jk}) \\ &+(N-3)u_6 \\ =&-(2N+1)u_3+u_2+u_4+(N-3)u_6.\end{aligned}$$

$$\begin{aligned}(4)\quad \frac{\partial}{\partial t}H_t(\omega_{ij},\omega_{kj}) =&\Delta H_t(\omega_{ij},\omega_{kj}) \\ =&-(3N-2)H_t(\omega_{ij},\omega_{kj})+\sum_{\alpha\neq i,j}[H_t(\omega_{\alpha j},\omega_{kj})+H_t(\omega_{i\alpha},\omega_{kj})] \\ =&-(3N-2)H_t(\omega_{ij},\omega_{kj})+H_t(\omega_{kj},\omega_{kj})+(N-3)u_4+H_t(\omega_{ik},\omega_{kj}) \\ &+(N-3)u_6 \\ =&-(2N+1)u_4+u_1+u_3+(N-3)u_6.\end{aligned}$$

$$
\begin{aligned}
(5)\quad \frac{\partial}{\partial t}H_t(\omega_{ij},\omega_{ik}) =& \Delta H_t(\omega_{ij},\omega_{ik})\\
=& -(3N-2)H_t(\omega_{ij},\omega_{ik}) + \sum_{\alpha\neq i,j}[H_t(\omega_{\alpha j},\omega_{ik}) + H_t(\omega_{i\alpha},\omega_{ik})]\\
=& -(3N-2)H_t(\omega_{ij},\omega_{ik}) + H_t(\omega_{kj},\omega_{ik}) + (N-3)u_6 + H_t(\omega_{ik},\omega_{ik})\\
&+ (N-3)u_5\\
=& -(2N+1)u_5 + u_1 + u_3 + (N-3)u_6.
\end{aligned}
$$

$$
\begin{aligned}
(6)\quad \frac{\partial}{\partial t}H_t(\omega_{ij},\omega_{kl}) =& \Delta H_t(\omega_{ij},\omega_{kl})\\
=& -(3N-2)H_t(\omega_{ij},\omega_{kl}) + \sum_{\alpha\neq i,j}[H_t(\omega_{\alpha j},\omega_{kl}) + H_t(\omega_{i\alpha},\omega_{kl})]\\
=& -(3N-2)H_t(\omega_{ij},\omega_{kl}) + H_t(\omega_{kj},\omega_{kl}) + H_t(\omega_{lj},\omega_{kl}) + (N-4)u_6\\
&+ H_t(\omega_{il},\omega_{kl}) + H_t(\omega_{ik},\omega_{kl}) + (N-4)u_6\\
=& -(N+6)u_6 + 2u_3 + u_4 + u_5.
\end{aligned}
$$

Note that equations (4) and (5) are the same and satisfy the same initial values. So $u_4(t) = u_5(t)$. We have the following system of ODEs:

$$
\begin{cases}
u_1'(t) = -(3N-2)u_1 + (N-2)u_4 + (N-2)u_5\\
u_2'(t) = -(3N-2)u_2 + 2(N-2)u_3\\
u_3'(t) = u_2 - (2N+1)u_3 + u_4 + (N-3)u_6\\
u_4'(t) = u_1 + u_3 - (2N+1)u_4 + (N-3)u_6\\
u_5'(t) = u_1 + u_3 - (2N+1)u_5 + (N-3)u_6\\
u_6'(t) = 2u_3 + u_4 + u_5 - (N+6)u_6\\
u_1(0) = 1, u_2(0) = u_3(0) = u_4(0) = u_5(0) = u_6(0) = 0.
\end{cases}
$$

From the symmetry of heat kernel, we have

$$
H_t(\omega_{ij},\omega_{ki}) = H_t(\omega_{ki},\omega_{ij}) = u_3(t).
$$

The solution of the above system is:

$$
\begin{aligned}
u_1(t) &= \frac{e^{-(N+2)t} + (N-1)e^{-2(N+1)t} + (N-1)e^{-2Nt} + (N^2-3N+1)e^{-3Nt}}{N(N-1)},\\
u_2(t) &= \frac{e^{-(N+2)t} + (N-1)e^{-2(N+1)t} - (N-1)e^{-2Nt} - e^{-3Nt}}{N(N-1)},\\
u_3(t) &= \frac{2(N-2)e^{-(N+2)t} + (N-1)(N-4)e^{-2(N+1)t} - (N-1)(N-2)e^{-2Nt} + 2e^{-3Nt}}{2N(N-1)(N-2)},\\
u_4(t) &= \frac{2(N-2)e^{-(N+2)t} + (N-1)(N-4)e^{-2(N+1)t} + (N-1)(N-2)e^{-2Nt} - 2(N^2-3N+1)e^{-3Nt}}{2N(N-1)(N-2)},\\
u_5(t) &= \frac{2(N-2)e^{-(N+2)t} + (N-1)(N-4)e^{-2(N+1)t} + (N-1)(N-2)e^{-2Nt} - 2(N^2-3N+1)e^{-3Nt}}{2N(N-1)(N-2)},\\
u_6(t) &= \frac{(N-2)e^{-(N+2)t} - 2(N-1)e^{-2(N+1)t} + Ne^{-3Nt}}{N(N-1)(N-2)}.
\end{aligned}
$$

We observe that $u_i(t)$, $i = 1, \ldots, 6$, can be re-written as

$$
u_i(t) = \frac{e^{-(N+2)t}}{N(N-1)}\Big(1 + \widetilde{u}_i(t)\Big), \qquad i = 1, \ldots, 6, \tag{6.1}
$$

where

$$
\begin{aligned}
\tilde{u}_1(t) &= (N-1)e^{-(N-2)t} + (N-1)e^{-Nt} + (N^2-3N+1)e^{-2(N-1)t},\\
\tilde{u}_2(t) &= -(N-1)e^{-(N-2)t} + (N-1)e^{-Nt} - e^{-2(N-1)t},\\
\tilde{u}_3(t) &= \frac{-(N-1)(N-2)e^{-(N-2)t} + (N-1)(N-4)e^{-Nt} + 2e^{-2(N-1)t}}{2(N-2)},\\
\tilde{u}_4(t) &= \frac{(N-1)(N-2)e^{-(N-2)t} + (N-1)(N-4)e^{-Nt} - 2(N^2-3N+1)e^{-2(N-1)t}}{2(N-2)},\\
\tilde{u}_5(t) &= \tilde{u}_4(t),\\
\tilde{u}_6(t) &= \frac{-2(N-2)e^{-Nt} + Ne^{-2(N-1)t}}{N-2}.
\end{aligned} \tag{6.2}
$$

Note that $\widetilde{u}_i(t)$ is bounded on $[0, \infty)$ and $\widetilde{u}_i(t) \to 0$ as $t \to \infty$. In fact, we can get more precise bounds as shown in the following lemma.

Lemma 6.1. *For $N \geq 4$, $i = 1, \ldots, 6$, and $t > 0$, we have*

$$
\big|\tilde{u}_i(t)\big| \leq N^2 - N - 1 \qquad \textit{and thus} \qquad \big|1 + \tilde{u}_i(t)\big| \leq N(N-1).
$$

Proof. Applying the triangle inequality to the expressions for $\tilde{u}_i(t)$ in (6.3), we get

$$\begin{aligned}
\big|\tilde{u}_1(t)\big| &= N^2 - N - 1,\\
\big|\tilde{u}_2(t)\big| &= 2N - 1,\\
\big|\tilde{u}_3(t)\big| &= \frac{(N-1)(N-4)}{2(N-2)} + \frac{N-1}{2} + \frac{1}{N-2} \le N,\\
\big|\tilde{u}_4(t)\big| &\le \max\left\{\frac{(N-1)(N-4)}{2(N-1)} + \frac{N-1}{2},\ \frac{N^2-3N+1}{N-2}\right\} \le N-1,\\
\big|\tilde{u}_5(t)\big| &= \big|\tilde{u}_4(t)\big| \le N-1,\\
\big|\tilde{u}_6(t)\big| &\le \max\left\{\frac{2(N-1)}{N-2},\ \frac{N}{N-2}\right\} \le 3.
\end{aligned} \tag{6.3}$$

For $N \ge 4$, $N^2 - 2N - 1$ dominates the other upper bounds and the assertion follows. □

The number of directed edges in K is equal to $\#V_1 = N(N-1)$. Define six $(0,1)$-matrices A_i, $i = 1, \dots, 6$, of order $\#V_1 \times \#V_1$ as follows. The rows and columns of each A_i are labeled by the edges in V_1, or equivalently by the forms w_{ij}. For $A_1, \dots, A_6$, entries equal to 1 are, respectively, (w_{ij}, w_{ij}), (w_{ij}, w_{ji}), (w_{ij}, w_{jk}), (w_{ij}, w_{kj}), (w_{ij}, w_{ik}), (w_{ij}, w_{kl}). Note that $H_t^K(w_{ij}, w_{jk}) = H_t^K(w_{jk}, w_{ij})$ and (w_{jk}, w_{ij}) can be identified with (w_{ij}, w_{ki}). So if a row is indexed by w_{ij} then an entry in the corresponding column is 1 if it is indexed by w_{jk} or w_{ki}, where i, j, k are distinct (see the matrix A_3 in the following example.) The following example illustrates the matrices A_i ,$i = 1, \dots, 6$, for the case $N = 4$.

Example 6.2. *For $N = 4$, we have*

$$\begin{aligned}
V_0 &= \{1, 2, 3, 4\}\\
V_1 &= \{12, 13, 14, 21, 23, 24, 31, 32, 34, 41, 42, 43\}.
\end{aligned}$$

$$A_1 = \begin{pmatrix}
1&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0\\
0&0&0&0&0&0&0&0&0&0&0&1
\end{pmatrix}, \quad A_2 = \begin{pmatrix}
0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&0\\
1&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0\\
0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&1\\
0&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&0&0
\end{pmatrix},$$

$$A_3 = \begin{pmatrix} 0&0&0&0&1&1&1&0&0&1&0&0 \\ 0&0&0&1&0&0&0&1&1&1&0&0 \\ 0&0&0&1&0&0&1&0&0&0&1&1 \\ 0&1&1&0&0&0&0&1&0&0&1&0 \\ 1&0&0&0&0&0&1&0&1&0&1&0 \\ 1&0&0&0&0&0&0&1&0&1&0&1 \\ 1&0&1&0&1&0&0&0&0&0&0&1 \\ 0&1&0&1&0&1&0&0&0&0&0&1 \\ 0&0&1&0&0&1&0&0&0&1&1&0 \\ 1&1&0&0&0&1&0&0&1&0&0&0 \\ 0&0&1&1&1&0&0&0&0&1&0&0 \\ 0&0&1&0&0&1&1&1&0&0&0&0 \end{pmatrix}, \quad A_4 = \begin{pmatrix} 0&0&0&0&0&0&0&1&0&0&1&0 \\ 0&0&0&0&1&0&0&0&0&0&0&1 \\ 0&0&0&0&0&1&0&0&1&0&0&0 \\ 0&0&0&0&0&0&1&0&0&1&0&0 \\ 0&1&0&0&0&0&0&0&0&0&0&1 \\ 0&0&1&0&0&0&0&0&1&0&0&0 \\ 0&0&0&1&0&0&0&0&0&1&0&0 \\ 1&0&0&0&0&0&0&0&0&0&1&0 \\ 0&0&1&0&0&1&0&0&0&0&0&0 \\ 0&0&0&1&0&0&1&0&0&0&0&0 \\ 1&0&0&0&0&0&0&1&0&0&0&0 \\ 0&1&0&0&1&0&0&0&0&0&0&0 \end{pmatrix},$$

$$A_5 = \begin{pmatrix} 0&1&1&0&0&0&0&0&0&0&0&0 \\ 1&0&1&0&0&0&0&0&0&0&0&0 \\ 1&1&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&1&1&0&0&0&0&0&0 \\ 0&0&0&1&0&1&0&0&0&0&0&0 \\ 0&0&0&1&1&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&1&1&0&0&0 \\ 0&0&0&0&0&0&1&0&1&0&0&0 \\ 0&0&0&0&0&0&1&1&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&1&1 \\ 0&0&0&0&0&0&0&0&0&1&0&1 \\ 0&0&0&0&0&0&0&0&0&1&1&0 \end{pmatrix}, \quad A_6 = \begin{pmatrix} 0&0&0&0&0&0&0&0&1&0&0&1 \\ 0&0&0&0&0&1&0&0&0&0&1&0 \\ 0&0&0&0&1&0&0&1&0&0&0&0 \\ 0&0&0&0&0&0&0&0&1&0&0&1 \\ 0&0&1&0&0&0&0&0&0&1&0&0 \\ 0&1&0&0&0&0&1&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0&1&0 \\ 0&0&1&0&0&0&0&0&0&1&0&0 \\ 1&0&0&1&0&0&0&0&0&0&0&0 \\ 0&0&0&0&1&0&0&1&0&0&0&0 \\ 0&1&0&0&0&0&1&0&0&0&0&0 \\ 1&0&0&1&0&0&0&0&0&0&0&0 \end{pmatrix}.$$

By using the matrices A_i and (6.3), we can write the heat kernel (matrix) on K as

$$H_t^K = \sum_{i=1}^{6} u_i(t) A_i = \sum_{i=1}^{6} \frac{e^{-(N+2)t}(1 + \widetilde{u}_i(t))}{N(N-1)} A_i \tag{6.4}$$

Lemma 6.3. *Let A_i be the matrices defined above, and let $\|A_i\|$ denote the maximum row sum norm of A_i. Then*

(a) $\|A_1\| = \|A_2\| = 1$*;*
(b) $\|A_3\| = 2(N-2)$*;*
(c) $\|A_4\| = \|A_5\| = N-2$*;*
(d) $\|A_6\| = (N-2)(N-3)$.

Consequently,

$$\max\left\{\|A_i\| : i = 1, \ldots, 6\right\} = \begin{cases} 2(N-2) & \textit{if } N = 4, \\ (N-2)(N-3) & \textit{if } N \geq 5. \end{cases} \tag{6.5}$$

Proof. (a) An entry of A_1 equal 1 if and only if its row and column are both indexed by ij, i.e., if and only if the entry is (ij, ij).

For A_2, we notice that if the row is indexed by ij, then an entry in that row is nonzero if and only if the column is indexed by ji. Hence the row sum is 1.

(b) We first note that if a row is indexed by ij, then an entry in that row is nonzero if the column is indexed by $jk, ik \in V_0 \setminus \{i, j\}$. There are $N-2$ such entries. Next, we note that since

$H_t^K(w_{ij}, w_{jk}) = H_t^K(w_{jk}, w_{ij})$, which can be identified with $H_t^K(w_{ij}, w_{ki})$, row ij has $N-2$ such entries. So the row sum is $2(N-2)$.

(c) For fixed ij, there are $N-2$ choices for k. Hence the row sum is $N-2$. Identifying $H_t^K(w_{kj}, w_{ij})$ with $H_t^K(w_{ij}, w_{kj})$ yields no other nonzero entries. The proof for A_5 is similar.

(d) For fixed ij, there are $N-2$ choices for k and $N-3$ choices for ℓ that give rise to a 1 in row ij. Thus the row sum is $(N-2)(N-3)$. Again, identifying $H_t^K(w_{i\ell}, w_{ij})$ with $H_t^K(w_{ij}, w_{k\ell})$ produces new possibilities.

Finally, (6.5) follows by observing that $2(N-2) \le (N-2)(N-3)$ if and only if $N \le 5$. □

Lemma 6.4. *For $i = 1, \dots, 6$, we have*

$$\left\|A_i(\Delta_1^{G^c} + L_0)\right\| \le \begin{cases} 4(N-2)(N^2-N-1) & \text{if } N = 4, \\ 2(N-2)(N-3)(N^2-N-1) & \text{if } N \ge 5. \end{cases}$$

Proof. Recall from Proposition 2.2 that $\Delta_n^{G^c} + L_{n-1} = \Delta_n^K - \Delta_n^G$. Hence

$$\begin{aligned} \|A_i(\Delta_1^{G^c} + L_0)\| &= \|A_i(\Delta_1^K - \Delta_1^G)\| \\ &\le \|A_i\| \, \|\Delta_1^K - \Delta_1^G\| \\ &\le \|A_i\| \, \|\Delta_1^K\|, \end{aligned}$$

where the last inequality is because the entries of Δ_1^K and Δ_1^G have the same sign.

Note that a non-diagonal entry of Δ_1^K is either 0 or 1, and a diagonal entry is $-(N(N-1)-1)$, negative of the degree of any vertex. Hence the maximal row sum of Δ_1^K is $2[N(N-1)-1]$. Now the lemma following by combining this and Lemma 6.3. □

Lemma 6.5. *For $i = 1, \dots, 6$, we have*

$$\left\|A_i(\Delta_1^{G^c} + L_0)\right\| \le \begin{cases} 4(N-2)(N^2-N-1) & \text{if } N = 4, \\ 2(N-2)(N-3)(N^2-N-1) & \text{if } N \ge 5. \end{cases}$$

Proof. Recall from Proposition 2.2 that $\Delta_n^{G^c} + L_{n-1} = \Delta_n^K - \Delta_n^G$. Hence

$$\begin{aligned} \|A_i(\Delta_1^{G^c} + L_0)\| &= \|A_i(\Delta_1^K - \Delta_1^G)\| \\ &\le \|A_i\| \, \|\Delta_1^K - \Delta_1^G\| \\ &\le \|A_i\| \, \|\Delta_1^K\|, \end{aligned}$$

where the last inequality is because the entries of Δ_1^K and Δ_1^G have the same sign.

Note that a non-diagonal entry of Δ_1^K is either 0 or 1, and a diagonal entry is $-(N(N-1)-1)$, negative of the degree of any vertex. Hence the maximal row sum of Δ_1^K is $2[N(N-1)-1]$. Now the lemma following by combining this and Lemma 6.3. □

Let $\mathcal{F}$ be the vector space of all real-valued functions on $[0,\infty)\times V_1$. Let $T:\mathcal{F}\to\mathcal{F}$ be a linear operator defined as

$$\begin{aligned}Tf_t(x) :&= -\int_0^t \Big(H^K_{t-s}(\Delta_1^{G^c}+L_0)\Big)f_s(x)\,ds\\ &= \frac{-e^{-(N+2)t}}{N(N-1)}\sum_{i=1}^{6}\int_0^t e^{(N+2)s}\Big(1+\widetilde{u}_i(t-s)\Big)A_i(\Delta_1^{G^c}+L_0)f_s(x)\,ds.\end{aligned}$$

We now give a sufficient condition for the series $\sum_{m=0}^{\infty}T^m$ to converge. Define

$$\gamma(N) := \begin{cases} \dfrac{-1}{N+2}\ln\Big(1-\dfrac{N+2}{24(N-2)(N^2-N-1)}\Big) & \text{if } N\le 4,\\ \dfrac{-1}{N+2}\ln\Big(1-\dfrac{N+2}{12(N-2)(N-3)(N^2-N-1)}\Big) & \text{if } N\ge 5.\end{cases} \tag{6.6}$$

Proposition 6.6. *Let $N\ge 4$. Then for all $t\in(0,\gamma(N))$, $\|T\|<1$.*

Proof. The proof is similar to that of Proposition 3.2.

$$\big\|Tf_t(x)\big\| \le \frac{e^{-(N+2)t}}{N(N-1)}\sum_{i=1}^{6}\int_0^t e^{(N+2)s}\big|1+\widetilde{u}_i(t-s)\big|\cdot\big\|A_i(\Delta_1^{G^c}+L_0)f_s(x)\big\|\,ds.$$

Using Lemmas 6.1 and 6.5 and letting

$$c := \sup\Big\{\big|1+\widetilde{u}_i(t-s)\big|\cdot\big\|A_i(\Delta_1^{G^c}+L_0)\big\| : i=1,\dots,6,\ 0<s\le t\Big\},$$

we have

$$\big\|Tf_t(x)\big\| \le \frac{e^{-(N+2)t}}{N(N-1)}\sum_{i=1}^{6}\int_0^t e^{(N+2)s}c\|f\|_\infty\,ds = \frac{6c(1-e^{-(N+2)t})}{N(N-1)(N+2)}\|f\|_\infty.$$

To complete the proof, we will only consider the case $N\ge 5$; the case $N=4$ is similar. According to Lemmas 6.1 and 6.5,

$$\frac{6c(1-e^{-(N+2)t})}{N(N-1)(N+2)} \le \frac{12(N-2)(N-3)(N^2-N-1)(1-e^{-(N+2)t})}{N+2},$$

which is less than 1 if

$$t < \frac{-1}{N+2}\ln\Big(1-\frac{N+2}{12(N-2)(N-3)(N^2-N-1)}\Big) = \gamma(N).$$

The proposition follows. ∎

Theorem 6.7. *Let $N\ge 4$, $\gamma(N)$ be as in* (6.6)*, $\tilde{u}_i$, $1\le i\le 6$, be defined as in* (6.3).

(a) *For all* $x, y \in V_1$ *and* $t \geq s \geq 0$,

$$
\begin{aligned}
H_t^G(x,y) &= H_t^K(x,y) - \int_0^t \Big(H_{t-s}^K (\Delta_1^{G^c} + L_0) H_s^G \Big)(x,y)\, ds, \\
&= H_t^K(x,y) - \frac{e^{-(N+2)t}}{N(N-1)} \sum_{i=1}^{6} \int_0^t e^{(N+2)s} \big(1 + \widetilde{u}_i(t-s)\big) A_i (\Delta_1^{G^c} + L_0) H_s^G(x,y)\, ds.
\end{aligned}
$$

(b) *For all* $t \in (0, \gamma(N))$,

$$
H_t^G(x,y) = \Big(\sum_{m=0}^{\infty} T^m \Big) H_t^K(x,y).
$$

Proof. (a) It follows from the proof of Proposition 2.3 that

$$
H_t^G(x,y) - H_t^K(x,y) = \int_0^t \sum_{z \in V_1} H_{t-s}^K(x,z)(\Delta_{1,z}^{G^c} + L_{0,z}) H_s^G(z,y)\, ds. \tag{6.7}
$$

By using the definitions of the matrices A_i (see (6.4)), we can write (2.14) as

$$
\begin{aligned}
&\sum_{z \in V_1} \Big(\sum_{i=1}^{6} u_i(t-s) A_i(x,z) \Big) (\Delta_{1,z}^{G^c} + L_{0,z}) H_s^G(z,y) \\
=& \sum_{i=1}^{6} u_i(t-s) \sum_{z \in V_1} A_i(x,z)(\Delta_{1,z}^{G^c} + L_{0,z}) H_s^G(z,y) \\
=& \sum_{i=1}^{6} u_i(t-s) \Big(A_i (\Delta_1^{G^c} + L_0) H_s^G \Big)(x,y) \\
=& \frac{e^{-(N+2)(t-s)}}{N(N-1)} \sum_{i=1}^{6} \Big(1 + \widetilde{u}_i(t-s) \Big) \Big(A_i (\Delta_1^{G^c} + L_0) H_s^G \Big)(x,y).
\end{aligned} \tag{6.8}
$$

Part (a) now follows by substituting (6.8) into (6.7).

Part (b) follows by combining Part (a) and Proposition 6.6 □

For 1-forms we cannot obtain an analogous expression for the subgragh heat kernel as the one in Corollary 3.4. The main reason is that for 0-forms, $TH_t^K(x,y)$ can be expressed explicitly as in (3.7). For 1-forms the expression is not so explicit and involves an integral, e.g., for $m = 1$,

$$
TH_t^K(x,y) := \frac{-e^{-(N+2)t}}{N(N-1)} \sum_{i=1}^{6} \int_0^t e^{(N+2)s} \Big(1 + \widetilde{u}_i(t-s) \Big) A_i (\Delta_{1,z}^{G^c} + L_{0,z}) H_s^K(x,y)\, ds.
$$

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References

[1] M. Berger, P. Gauduchon, and E. Mazet, Le spectre d'une variété riemannienne, *Lecture Notes in Mathematics* **194**, Springer-Verlag, Berlin-New York 1971.

[2] G. Chinta, G. J. Jorgenson, and A. Karlsson, Heat kernels on regular graphs and generalized Ihara zeta function formulas, *Monatsh. Math.* **178** (2015), 171–190.

[3] F. R. K. Chung, *Spectral graph theory*, CBMS Regional Conference Series in Mathematics, **92**, American Mathematical Society, Providence, RI, 1997.

[4] F. K. R. Chung and S.-T. Yau, A combinatorial trace formula, *Tsing Hua lectures on geometry & analysis (Hsinchu, 1990–1991)*, 107–116, Int. Press, Cambridge, MA, 1997.

[5] F. Chung and S.-T. Yau, Coverings, heat kernels and spanning trees, *Electron. J. Combin.* **6** (1999), Research Paper 12, 21 pp.

[6] A. Grigor'yan, Y. Lin, Y. Muranov, and S.-T. Yau, Homotopy theory for digraphs, *Pure and Appl. Math. Q.* **10** (2014), 619–674.

[7] A. Grigor'yan, Y. Lin, Y. Muranov, and S.-T. Yau, Cohomology of digraphs and (undirected) graphs, *Asian J. Math.* **19** (2015), 887–932.

[8] A. Grigoryan and A. Telcs, Sub-Gaussian estimates of heat kernels on infinite graphs, *Duke Math. J.* **109** (2001), 451–510.

[9] O. Knill, A graph theoretical Gauss-Bonnet-Chern theorem, arXiv preprint arXiv:1111.5395, 2011.

[10] O. Knill, The McKean-Singer Formula in Graph Theory, arXiv preprint arXiv:1301.1408, 2013.

[11] H. P. McKean, Jr. and I. M. Singer, Curvature and the eigenvalues of the Laplacian, *J. Differential Geometry*, **1** (1967), 43–69.

[12] S. Minakshisundaram, Eigenfunctions on Riemannian manifolds, *J. Indian Math. Soc. (N.S.)* **17** (1953), 159–165.

[13] S. Minakshisundaram and A. Pleijel, Some properties of the eigenfunctions of the Laplace-operator on Riemannian manifolds, *Canadian J. Math.* **1** (1949), 242–256.

[14] V. K. Patodi, Curvature and the eigenforms of the Laplace operator, *J. Differential Geometry* **5** (1971), 233–249.

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