The parametrix construction of the heat kernel on a graph *

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Dedicated to Steven G. Krantz, for his 70th birthday, and with appreciation for his many contributions to the mathematical community.

Abstract

In this paper we develop the parametrix approach for constructing the heat kernel on a graph G. In particular, we highlight two specific cases. First, we consider the case when G is embedded in a Eulidean domain or manifold Ω, and we use a heat kernel associated to Ω to obtain a formula for the heat kernel on G. Second, we consider when G is a possibly infinite subgraph of a larger graph $\widetilde{G}$, and we obtain a formula for the heat kernel on G from the heat kernel on $\widetilde{G}$ restricted to G.

1 Introduction

A heat kernel is the fundamental solution to a heat equation in a domain, manifold or graph, which may be subject to certain boundary conditions. Heat kernels have proved useful when studying a variety of problems, from geometry and topology to combinatorics and mathematical physics; see, for example [Gr09] or [JoLa01] for some general discussion as to the many manifestations of heat kernel techniques throughout mathematics. Algebraically, the heat kernel can be viewed as a generating function of the spectrum of the Laplace operator, in instances when its spectrum is discrete.

In this article we will prove a construction of the heat kernel on graphs analogous to the parametrix construction in Riemannian geometry, [MP49, Mi49, Ch84, Ro97]. The parametrix approach plays an important role in geometry and in varied applications such as machine learning [LL05] and quantum field theory [Av01]. In brief, this approach to constructing the heat kernel on a Riemannian manifold M begins with an initial approximation which could, for example, come from the Euclidean heat kernel patched together on local charts. This is then refined through an iterative process. The successive refinements provide an increasingly precise small time asymptotic expansion of the heat kernel.

We will describe the construction of the heat kernel on a finite graph by starting with a general parametrix. We pay particular attention to situations in which a finite graph G is embedded in an ambient space, which may be a domain in $\mathbb{R}^n$, a manifold or another larger graph. Then we may take our initial approximation in the parametrix construction to be the heat kernel on the ambient space. This allows us to extend our results to construction of the heat kernel on infinite subgraphs with a finite boundary. In Example 15 below we will use the

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heat kernel on $\tilde{G} = \mathbb{Z}$, when viewed as a 2-regular tree, as a parametrix and prove that the heat kernel on the discrete half-line $G = \mathbb{Z}_{\geq 0}$ is given by

$$H_{\mathbb{Z}_{\geq 0}}(v, w; t) = e^{-2t}(I_{v-w}(2t) + I_{v+w+1}(2t)) \text{ for all } v, w \in \mathbb{Z}_{\geq 0} \text{ and } t \geq 0,$$

where I_ν denotes the I-Bessel function.

A similar construction in the special case when G is embedded in a complete graph is considered in [LNY21]. In Section 6 below we relate our method to the approach in [LNY21] and show how our construction implies one of the main results of [LNY21].

Let us now be more specific in describing the results of this article. Let G be a finite, edge-weighted graph with finite vertex set VG and nonnegative weight function $w : VG \times VG \to [0, \infty), w \mapsto w_{xy}$. When $w_{xy} = 0$ we say there is no edge between x and y. Furthermore, we assume the symmetry $w_{xy} = w_{yx}$ holds for all $x, y \in VG$. This data defines the Laplace operator Δ_G on functions $f : VG \to \mathbb{C}$ by

$$\Delta_G f(x) = \sum_{y \in VG} (f(x) - f(y))w_{xy}.$$

Note that the sum in fact is taken over the neighbors of x, that is, over the vertices y with weight $w_{xy} > 0$. The *heat kernel* on the graph G associated to the weighted graph Laplacian Δ_{G,v_1} acting on functions in the first variable v_1, is the unique solution $H_G(v_1, v_2; t)$ to the differential equation

$$\left(\Delta_{G,v_1} + \frac{\partial}{\partial t}\right) H_G(v_1, v_2; t) = 0$$

with the property that

$$\lim_{t \to 0} H_G(v_1, v_2; t) = \begin{cases} 1 \text{ if } v_1 = v_2 \\ 0 \text{ if } v_1 \neq v_2. \end{cases}$$

For the proof of the existence and uniqueness of the heat kernel on G, we refer to [Do84] and [DM06]. We do not normalize the Laplacian $\Delta_G f(x)$ by dividing the sum defining it by the weighted degree $\mu(x) = \sum_{y \in VG} w_{xy}$ of x; this normalization appears mostly when discussing stochastic properties of graphs, see e.g. [Wo21] and the extensive bibliography there. However, the parametrix construction of the heat kernel given in our main result Theorem 5 can be carried out in the same manner for the "normalized" Laplacian.

After we give a reasonably general construction in Theorem 5, we then explain in Proposition 6 how to obtain a parametrix of higher order. We will highlight the following two special cases.

1. When the set VG is a subset of a bounded domain Ω in $\mathbb{R}^N$, we show that the parametrix for the heat kernel on G can be obtained from the heat kernel on Ω and a certain partition of unity depending upon a (Dirichlet-)Voronoĭ decomposition of Ω induced by G.

2. When G is a finite or infinite subgraph of a graph $\tilde{G}$, we prove that the heat kernel on $\tilde{G}$ can be used as a parametrix of order zero in the construction of the heat kernel on G, under the technical assumption that the boundary ∂G of G when viewed as a subgraph of $\tilde{G}$ has a finite number of vertices.

Any new expression for the heat kernel is potentially a source for interesting new identities, which occurs since in the case when the heat kernel is unique. For example, when studying continuous functions on the continuous circle, one can write the heat kernel either through its spectral expansion or through the periodization of the heat kernel on the covering space. In doing so, one immediately obtains a classical theta inversion formula, which itself is logically equivalent to the one-variable Poisson summation formula. A similar argument in the setting of compact hyperbolic Riemann surfaces yields a quick proof of the Selberg trace formula; see Remark 3.3 of [GJ18]. In the case of a heat kernel on a discrete circle with N points, then similar considerations in [KN06] lead to "heat kernel proofs" of I-Bessel identities. See also [Gr22] and [CHJSV23] for proofs of trigonometric identities using the uniqueness of the discrete-time heat kernel on a discrete circle with N points.

With this in mind, in Example 17 we specialize our general result to the discrete half-line $\mathbb{Z}_{\geq 0}$ with a Dirichlet boundary condition. We define the time convolution of I-Bessel functions

$$\left(I_x * I_y\right)(t) = \int_0^t I_x(\tau) I_y(t-\tau) d\tau. \tag{1}$$

Then the parametrix construction of the heat kernel on $\mathbb{Z}_{\geq 0}$ yields the identity

$$I_{x+y}(t) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{2^{\ell+1}} \left(I_1^{*\ell} * I_{x-1} * I_y\right)(t) \tag{2}$$

where $I_1^{*\ell}$ denotes the ℓ-fold convolution of I_1 itself. This identity can be confirmed directly by comparing the Laplace transform of both sides.

The paper is organized as follows. In Section 2 we develop various analytic results which are needed in our study. Section 3 contains the details of the general parametrix construction and its refinement. In Section 4 we relate the heat kernel of a graph embedded in a domain with the heat kernel of the domain. Corollary 10 is particularly interesting since it gives a precise relation between the graph heat kernel on a graph G which is embedded in a domain Ω in terms of the geometric heat kernel associated to Ω, up to $O(t^2)$ for small time t. Section 5 deals with derivation of expressions for the heat kernel in a general subgraph case. In Section 6 we show that our general result, applied to the setting of the complete graph on N vertices yields some of the main results from Section 3 of [LNY21]. We also give an alternative formulation for those results and explicitly compute the heat kernel on the graph obtained by removing a single edge from the complete graph. An example of an infinite subgraph is treated in Section 7. In Section 8, we show how to construct the Dirichlet heat kernel on a subgraph G of a finite or infinite graph, assuming that boundaries of G and $G \setminus \partial G$ are finite. An example in this section yields the I-Bessel function identity (2).

2 Convolution on a graph

Let G be a finite weighted graph as above with vertex set VG of cardinality $|VG|$. Let $F_1, F_2 : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$. Assume further that for $i = 1, 2$ and fixed vertices v_1, v_2, the functions $F_i(v_1, v_2; t)$ are integrable as functions of t on every interval $(0, b]$ with $b > 0$. The *convolution* of functions F_1 and F_2 is defined to be

$$(F_1 * F_2)(v_1, v_2; t) := \int_0^t \sum_{v \in VG} F_1(v_1, v, t-r) F_2(v, v_2; r) dr. \tag{3}$$

When thinking of F_1 and F_2 as operators on $L^2(VG)$, or equivalently as $|VG| \times |VG|$ matrices, we may simply write

$$(F_1 * F_2)(t) := \int_0^t F_1(t-r) \circ F_2(r) dr. \tag{4}$$

The above convolution is not commutative in general but it is associative. Specifically, for any three functions $F_i(v_1, v_2; t)$, $i = 1, 2, 3$, $F_i : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$ which are integrable as functions of t on every interval $(0, b]$, $b > 0$ for all $v_1, v_2 \in VG$, we have

$$[(F_1 * F_2) * F_3](v_1, v_2; t) = [F_1 * (F_2 * F_3)](v_1, v_2; t). \tag{5}$$

Remark 1. There are two notions of convolution which are used in this paper: the two-variable vertex and time convolution (3) defined in this section and a one-variable time convolution as in (1). The latter is used only in Example 17 of Section 8 and we hope no confusion will arise from using the same symbol $*$ to denote both types of convolution.

We have the following lemma.

Lemma 2. *Let $F_1, F_2 : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$ be as above. For some $t_0 > 0$, assume there exist constants C_1, C_2 and integers $k, \ell \geq 0$ such that for all $0 < t < t_0$ and $v_1, v_2 \in VG$, we have*

$$|F_1(v_1, v_2; t)| \leq C_1 t^k \quad \text{and} \quad |F_2(v_1, v_2; t)| \leq C_2 t^\ell.$$

Then, for all $v_1, v_2 \in VG$ we have

$$|(F_1 * F_2)(v_1, v_2; t)| \leq C_1 C_2 |VG| \frac{k!\ell!}{(k + \ell + 1)!} t^{k+\ell+1} \quad \text{for } 0 < t < t_0.$$

In particular, if $k = 0$ then

$$|(F_1 * F_2)(v_1, v_2; t)| \leq C_1 C_2 |VG| \frac{t^{\ell+1}}{\ell + 1} \quad \text{for all } v_1, v_2 \in VG \text{ and } 0 < t < t_0.$$

Proof. The proof is immediate from the definition of the convolution and the formula for the Euler beta function, namely that

$$\int_0^t r^k (t - r)^\ell \, dr = \frac{k!\ell! t^{k+\ell+1}}{(k + \ell + 1)!}.$$

□

For any positive integer ℓ and any function $f = f(v_1, v_2; t) : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$ which is integrable in t on every interval $(0, b]$, $b > 0$ for all $v_1, v_2 \in VG$, we can inductively define the ℓ-fold convolution $(f)^{*\ell}(v_1, v_2; t)$ by setting $(f)^{*1}(v_1, v_2; t) = f(v_1, v_2; t)$ and, for $\ell \geq 2$ we put

$$(f)^{*\ell}(v_1, v_2; t) := \left((f)^{*(\ell-1)} * f\right)(v_1, v_2; t).$$

Note that in the last definition the order is not important because the convolution operator is associative.

With this notation we have the following lemma.

Lemma 3. *Let $f = f(v_1, v_2; t) : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$. Assume that for all $v_1, v_2 \in VG$ and $t_0 \in \mathbb{R}_{>0}$, the function $f(v_1, v_2; \cdot)$ is integral on the interval $(0, t_0]$. Assume further there exists a constant C and integer $k \geq 0$ such that*

$$f(v_1, v_2; t) \leq C t^k \quad \text{for all } v_1, v_2 \in VG \text{ and } 0 < t < t_0.$$

Then the series

$$\sum_{\ell=1}^{\infty} (-1)^\ell (f)^{*\ell}(v_1, v_2; t) \tag{6}$$

converges absolutely and uniformly on every compact subset of $VG \times VG \times \mathbb{R}_{>0}$. In addition, we have that

$$\left(f * \sum_{\ell=1}^{\infty}(-1)^{\ell}(f)^{*\ell}\right)(v_1, v_2; t) = \sum_{\ell=1}^{\infty}(-1)^{\ell}(f)^{*(\ell+1)}(v_1, v_2; t) \tag{7}$$

and,

$$\sum_{\ell=1}^{\infty}\left|(f)^{*\ell}(v_1, v_2; t)\right| = O(t^k) \quad \text{as } t \to 0. \tag{8}$$

Proof. With the stated assumptions, together with Lemma 2, we have that

$$|(f * f)(v_1, v_2; t)| \leq C^2|VG|(k!)^2\frac{t^{2k+1}}{(2k+1)!}. \tag{9}$$

Similarly, by induction for $\ell \geq 1$ we have the bound that

$$\left|(f^{*(\ell)})(v_1, v_2; t)\right| \leq (Ck!)^{\ell}|VG|^{\ell-1}\frac{t^{\ell k+\ell-1}}{(\ell k+\ell-1)!}. \tag{10}$$

The assertion regarding the convergence of (6) now follows from the Weierstrass criterion.

Fix $t > 0$. By reasoning as above, it is easy to deduce that the series on the right-hand side of (7) converges absolutely. Therefore, we may integrate the equation

$$\left(f * \sum_{\ell=1}^{\infty}(-1)^{\ell}(f)^{*\ell}\right)(v_1, v_2; t) = \int_0^t \sum_{v \in VG}\left(f(v_1, v, t-r)\sum_{\ell=1}^{\infty}(-1)^{\ell}(f)^{*\ell}(v, v_2; r)\right) dr$$

termwise to establish (7). Finally, the assertion in (8) follows by combining (6), (10), and Lemma 2.

□

3 The parametrix construction of the heat kernel on G

We repeat and expand on some notation from the introduction. Let G be a finite weighted graph with vertex set VG and edge weight function w_{xy} for vertices x, y. The Laplace operator Δ_G acting on functions $f : VG \to \mathbb{C}$ is defined by

$$\Delta_G f(x) = \sum_{y \in VG}(f(x) - f(y))w_{xy} \tag{11}$$

and the heat operator L on the graph is defined by

$$L = \Delta_G + \frac{\partial}{\partial t}. \tag{12}$$

The heat kernel H_G on G associated to the Laplacian Δ_G is the unique solution $H_G : VG \times VG \times [0, \infty)$ to the differential equation

$$L_{v_1}H_G(v_1, v_2; t) = 0$$

with the property that

$$H_G(v_1, v_2; 0) = \begin{cases} 1 & \text{if } v_1 = v_2 \\ 0 & \text{if } v_1 \neq v_2. \end{cases}$$

The subscript v_1 on L_{v_1} indicates the sum associated to the Laplacian, as in (11) is over neighbors of v_1 which is the first space variable. A *parametrix* for the heat operator on G is any continuous function $H : VG \times VG \times [0, \infty)$ which is smooth on $VG \times VG \times (0, \infty)$ and satisfies the following two properties.

1. For all $v_1, v_2 \in VG$,

$$H(v_1, v_2; 0) = \lim_{t \to 0} H(v_1, v_2; t) = \begin{cases} 1 & \text{if } v_1 = v_2 \\ 0 & \text{if } v_1 \neq v_2 \end{cases} \tag{13}$$

2. The function $L_{v_1} H(v_1, v_2; t)$ extends to a continuous function on $VG \times VG \times [0, \infty)$.

We say the parametrix H is of order k if for some integer $k \geq 0$,

$$|L_{v_1} H(v_1, v_2; t)| = O(t^k) \quad \text{as } t \to 0.$$

Lemma 4. *Let H be a parametrix for the heat operator on G. Let $f = f(v_1, v_2; t) : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$ be continuous in t and bounded for all $v_1, v_2 \in VG$. Then*

$$L_{v_1}(H * f)(v_1, v_2; t) = f(v_1, v_2; t) + (L_{v_1} H * f)(v_1, v_2; t)$$

for all $v_1, v_2 \in VG$ and $t \in \mathbb{R}_{>0}$.

Proof. For any $t > 0$ we have

$$L_{v_1}(H * f) = \frac{\partial}{\partial t}(H * f) + \Delta_{G,v_1}(H * f) = \frac{\partial}{\partial t}(H * f) + (\Delta_{G,v_1} H) * f. \tag{14}$$

By the Leibniz integration formula, the first term on the right hand side of (14) is equal to

$$\begin{aligned} &\frac{\partial}{\partial t} \int_0^t \sum_{v \in VG} H(v_1, v; t - r) f(v, v_2; r) dr \\ &= \sum_{v \in VG} H(v_1, v; 0) f(v, v_2; t) + \int_0^t \sum_{v \in VG} \frac{\partial}{\partial t} H(v_1, v; t - r) f(v, v_2; r) dr \\ &= f(v_1, v_2; t) + (\frac{\partial}{\partial t} H * f)(v_1, v_2; t). \end{aligned}$$

Therefore,

$$\begin{aligned} L_{v_1}(H * f)(v_1, v_2; t) &= \frac{\partial}{\partial t}(H * f)(v_1, v_2; t) + (\Delta_{G,v_1} H * f)(v_1, v_2; t) \\ &= f(v_1, v_2; t) + (\frac{\partial}{\partial t} H * f)(v_1, v_2; t) + (\Delta_{G,v_1} H * f)(v_1, v_2; t) \\ &= f(v_1, v_2; t) + (L_{v_1} H * f)(v_1, v_2; t), \end{aligned}$$

as claimed. □

With all this, we now can state the main theorem in this section

Theorem 5. *Let H be a parametrix of order $k \geq 0$. For $v_1, v_2 \in VG$ and $t \in \mathbb{R}_{\geq 0}$ define*

$$F(v_1, v_2; t) := \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} H)^{*\ell}(v_1, v_2; t). \tag{15}$$

Then the series (15) *converges absolutely and uniformly on every compact subset of $VG \times VG \times \mathbb{R}_{\geq 0}$. Furthermore, the heat kernel H_G on G associated to graph Laplacian Δ_{G,v_1} is given by*

$$H_G(v_1, v_2; t) = H(v_1, v_2; t) + (H * F)(v_1, v_2; t) \tag{16}$$

with

$$(H * F)(v_1, v_2; t) = O(t^{k+1}) \quad \text{as } t \to 0.$$

Proof. Set

$$\tilde{H}(v_1, v_2; t) := H(v_1, v_2; t) + (H * F)(v_1, v_2; t).$$

From the characterizing properties of the heat kernel

$$\lim_{t \to 0} \widetilde{H}(v_1, v_2; t) = \lim_{t \to 0} H(v_1, v_2; t) = \delta_{v_1 = v_2},$$

it suffices to show that

$$L_{v_1} \tilde{H}(v_1, v_2; t) = 0 \quad \text{and} \quad \lim_{t \to 0} \tilde{H}(v_1, v_2, t) = \delta_{v_1 = v_2}. \tag{17}$$

By Lemma 3, the series $F(v_1, v_2; t)$ defined in (15) converges uniformly and absolutely and has order $O(t^k)$ as $t \to 0$. Since H is bounded on any finite interval, Lemma 2 then yields the asymptotic

$$(H * F)(v_1, v_2; t) = O(t^{k+1}) \quad \text{as } t \to 0.$$

In particular,

$$\lim_{t \to 0} \widetilde{H}(v_1, v_2; t) = \lim_{t \to 0} H(v_1, v_2; t) = \delta_{v_1 = v_2}.$$

It remains to prove the vanishing of $L_{v_1} \tilde{H}$ in (17). For this, we can apply Lemma 4 to get that

$$\begin{aligned} L_{v_1} \tilde{H}(v_1, v_2; t) &= L_{v_1}(H)(v_1, v_2; t) + L_{v_1}(H * F)(v_1, v_2; t) \\ &= L_{v_1}(H)(v_1, v_2; t) + \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} H)^{*\ell}(v_1, v_2; t) \\ &\quad + (L_{v_1} H) * \left(\sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} H)^{*(\ell)} \right) (v_1, v_2; t) \\ &= L_{v_1}(H)(v_1, v_2; t) + \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} H)^{*\ell}(v_1, v_2; t) \\ &\quad + \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} H)^{*(\ell+1)}(v_1, v_2; t) \\ &= 0, \end{aligned}$$

where we used absolute convergence of the series defining $F(v_1, v_2; t)$ to change the order of summation. This completes the proof. □

The construction of the heat kernel on G begins by starting with a reasonably general function as a parametrix. This method can be further refined, depending upon the properties of the parametrix. For example, if an order zero parametrix $H(v_1, v_2; t)$ is $n+1$ times continuously differentiable in t for all $v_1, v_2 \in VG$, then one may define a function $H_n(v_1, v_2; t)$ which is a parametrix of order n for the heat operator on G. This following proposition establishes this assertion.

Proposition 6. *With the notation as above, let H be a parametrix of order zero for the heat operator on the graph G. Assume further that $H(v_1, v_2; t)$ is $n+1$ times continuously differentiable in t for all $v_1, v_2 \in VG$. For $j = 1, \ldots, n$, let $u_j : VG \times VG \to \mathbb{R}$ be a sequence of functions which are defined inductively as follows. Let*

$$u_1(v_1, v_2) := (L_{v_1} H)(v_1, v_2; 0),$$

and for $2 \leq j \leq n$ set

$$u_j(v_1, v_2) = \frac{\partial^{j-1}}{\partial t^{j-1}} (L_{v_1} H)(v_1, v_2; t)\Big|_{t=0} - \Delta_{G,v_1} u_{j-1}(v_1, v_2).$$

Then, the function

$$H_n(v_1, v_2; t) := H(v_1, v_2; t) - \sum_{j=1}^{n} \frac{t^j}{j!} u_j(v_1, v_2)$$

is a parametrix of order n for the heat operator L_{v_1} on G.

Proof. Trivially, $\lim_{t \to 0} H_n(v_1, v_2; t) = \delta_{v_1 = v_2}$ and $(L_{v_1} H_n)(v_1, v_2; t)$ extends to a continuous function on $VG \times VG \times [0, \infty)$. So then, it remains to determine the asymptotic behavior of $(L_{v_1} H_n)(v_1, v_2; t)$ as $t \to 0$.

By assumption, the parametrix $H(v_1, v_2; t)$ is $n + 1$ times continuously differentiable in t. Hence, for any two points $v_1, v_2 \in VG$, we have the expansion that

$$(L_{v_1} H)(v_1, v_2; t) = \sum_{j=0}^{n-1} \frac{t^j}{j!} \frac{\partial^j}{\partial t^j} (L_{v_1} H)(v_1, v_2; t)\Big|_{t=0} + O(t^n) \quad \text{as } t \to 0.$$

The implicit constant in the term $O(t^n)$ depends on v_1, v_2, and it is uniform in t for all t in some interval $(0, \delta)$. Therefore,

$$\begin{aligned}(L_{v_1} H_n)(v_1, v_2; t) &= (L_{v_1} H)(v_1, v_2; t) - \sum_{j=1}^{n} \frac{t^j}{j!} \Delta_{G,v_1} u_j(v_1, v_2) - \sum_{j=1}^{n} \frac{t^{j-1}}{(j-1)!} u_j(v_1, v_2) \\ &= \sum_{j=1}^{n} \frac{t^{j-1}}{(j-1)!} \left(\frac{\partial^{j-1}}{\partial t^{j-1}} (L_{v_1} H)(v_1, v_2; t)\Big|_{t=0} - u_j(v_1, v_2) - \Delta_{G,v_1} u_{j-1}(v_1, v_2) \right) \\ &\qquad + O(t^n) = O(t^n) \ \text{ as } \ t \to 0,\end{aligned}$$

where we have set that $u_0 \equiv 0$. With this, the proof of the assertion is complete. □

Remark 7. In (16), the function $H(v_1, v_2; t)$ is a parametrix, so it is required to satisfy the reasonably weak conditions given in its definition. In particular, one does not use any information about the edge structure associated to the graph. One incorporates the finer information regarding the edge data through the Laplacian, which is used to form the Neumann series (15). In this regard, the parametrix construction of the heat kernel on a graph, as given in Theorem 5 is easier than the parametrix construction for the heat kernel in the setting of Riemannian geometry (see, for example, Chapter IV of [Ch84], page 149) where the Laplacian is necessary in the construction of the parametrix.

4 Graphs embedded in a domain

Let us assume that a graph G is embedded in a Riemannian domain Ω. In this section, we will show one way in which the Riemannian heat kernel on Ω can be used to construct the graph heat kernel on G. In effect, we define a parametrix on the graph by computing an average of the heat kernel from Ω over neighborhoods of the vertices of G. We then employ Theorem 5. Certainly, there are other means by which one could define a parametrix. However, we find it appealing to develop a direct connection between the Riemannian heat kernel on Ω and the graph heat kernel on G.

Let $\Omega \subset \mathbb{R}^N$ be a bounded domain with C^∞ boundary $\partial\Omega$. The Laplacian on Ω is defined through its action on twice continuously differentiable functions f on Ω as

$$\Delta_\Omega f(x) = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} f(x).$$

Let $K_\Omega(x, y; t)$ denote a heat kernel on Ω, meaning the fundamental solution to the equation

$$(\Delta_\Omega + \partial_t)K(x, y; t) = 0$$

on $\Omega \times \Omega \times (0, \infty)$ subject to the initial condition

$$\lim_{t \to 0} K(x, y; t) = \delta_x,$$

where δ_x is the Dirac delta mass concentrated at x. For definiteness we assume that $K_\Omega(x, y; t)$ satisfies a Dirichlet boundary condition, but this will play no role in our construction and any reasonable alternative boundary condition may be assumed. We assume that Ω is fixed and will suppress the subscript Ω and denote a the heat kernel on Ω simply by $K(x, y; t)$. Heat kernels with different boundary condition are, of course, different; however, for our construction we can take any one.

Let G be a graph embedded in Ω, in the sense that $VG \subset \Omega$. Let d denote the Euclidean distance on Ω and let m be the Lebesgue measure also denoted dx below. For any vertex v in G we let

$$N(v) = \{x \in \Omega : d(x, v) < d(x, v') \text{ for all } v' \in VG\}$$

be the (Dirichlet-) Voronoĭ decomposition of Ω induced by VG. In words, $N(v)$ is the set of points in Ω closer to v than any other vertex in VG. The collection of sets $\{N(v) : v \in VG\}$ are disjoint, by construction, and non-empty since $v \in N(v)$. Each set is open, thus measurable. We assume that VG is embedded in Ω in such a way that all sets $N(v)$ in the Voronoĭ decomposition are path-connected. We denote by μ_v the measure of $N(v)$. For example, if Ω is convex, then each set $N(v)$ is open and convex.

The set

$$H(v, v') := \{x \in \mathbb{R}^N : d(x, v) = d(x, v') : v, v' \in VG\}$$

is a union of hyperplanes in $\mathbb{R}^N$, hence a measure zero set. The set $\Omega \setminus \bigcup_{v \in VG} N(v)$ is a subset of $H(v, v')$, hence is also a set of measure zero.

For any $\delta > 0$ and $v \in VG$, define the set

$$N_\delta(v) := \{x \in N(v) : d(x, \partial N(v)) < \delta\},$$

where $\partial N(v)$ stands for the boundary of $N(v)$. For an arbitrary and fixed $\epsilon > 0$, we choose $\delta > 0$ which depends on ϵ and G such that

$$N(v) \setminus N_\delta(v) \neq \emptyset \quad \text{and} \quad m(N_\delta(v)) < \epsilon/|VG| \text{ for all } v \in VG.$$

For such a fixed $\epsilon > 0$, let us introduce a family of C^{∞}-functions $\eta_v : \Omega \to [0, \infty)$, indexed by $v \in VG$, which satisfy the following properties.

(a) For all $v \in VG$ one has $\mathrm{supp}(\eta_v) \subseteq N(v)$, meaning $\eta_v(x) = 0$ whenever $x \notin N(v)$.

(b) We have that $\eta_v(x) \equiv 1$ for all $x \in N(v) \setminus N_\delta(v)$ and $\eta_v(x) \equiv 0$ for all $x \in N_{\delta/2}(v)$.

(c) For all $v \in VG$, we have that

$$\int_{\Omega} \eta_v(x)^2 dx = \mu_v = m(N(v)).$$

In words, the function η_v is equal to one on $N(v) \setminus N_\delta(v)$, equal to zero outside $N(v) \setminus N_{\delta/2}(v)$, increases from one and then decrease to zero on $N_\delta(v) \setminus N_{\delta/2}(v)$ so that one has the integral condition (c). It is an elementary exercise in real analysis to construct such a family of functions. Later, we will use the relation

$$\int_{\Omega} \eta_v(x)\, dx \leq \int_{N(v)} 1 \cdot \eta_v(x) dx \leq \left(\int_{N(v)} 1 dx \right)^{1/2} \left(\int_{N(v)} \eta_v^2(x) dx \right)^{1/2} = \mu_v \tag{18}$$

where we used (a) and (c) above, together with the Cauchy-Schwartz inequality.

With this notation, we can use a heat kernel $K(x, y; t)$ on Ω to construct a parametrix of any order $k \geq 0$ for the heat kernel on the graph G. The details are as follows. For any $v_1, v_2 \in VG$ and $t > 0$, define

$$H_0(v_1, v_2; t) = \frac{1}{\sqrt{\mu_{v_1} \mu_{v_2}}} \int_{N(v_1)} \int_{N(v_2)} K(x, y; t) \eta_{v_1}(x) \eta_{v_2}(y) dy dx. \tag{19}$$

From the known properties of K, and from the smoothness of the family η_v for $v \in VG$, the function (19) is infinitely differentiable in t. Moreover, for each $v \in VG$ the function

$$u_v(x; t) := \int_{N(v)} K(x, y; t) \eta_v(y) dy = \int_{\Omega} K(x, y; t) \eta_v(y) dy$$

is a solution to the initial value problem

$$\left(\Delta_\Omega + \frac{\partial}{\partial t} \right) u_v(x; t) = 0 \quad \text{for} \quad (x, t) \in \Omega \times (0, \infty) \tag{20}$$

with

$$u_v(x; 0) = \eta_v(x) \quad \text{for} \quad x \in \Omega. \tag{21}$$

Proposition 8. *Assume the notation as above.*

(i) For all $v_1, v_2 \in VG$, we have that

$$\lim_{t \to 0} H_0(v_1, v_2; t) = \begin{cases} 1 & \text{if } v_1 = v_2 \\ 0 & \text{if } v_1 \neq v_2 \end{cases} \tag{22}$$

(ii) For any $k \geq 0$ all $v_1, v_2 \in VG$, there is a constant $C_k(v_1, v_2)$ such that for all $t > 0$, we have that

$$\left| \frac{\partial^k}{\partial t^k} H_0(v_1, v_2; t) \right| \leq C_k(v_1, v_2) \quad \text{as } t \to 0. \tag{23}$$

Proof. (i) From the definition (19) of H_0, we have that

$$\lim_{t\to 0} H_0(v_1, v_2; t) = \lim_{t\to 0} \frac{1}{\sqrt{\mu_{v_1}\mu_{v_2}}} \int\limits_{N(v_1)} \eta_{v_1}(x) u_{v_2}(x; t) dx.$$

Since all sets are bounded and have finite volume, the dominated convergence theorem implies that

$$\lim_{t\to 0} \int\limits_{N(v_1)} \eta_{v_1}(x) u_{v_2}(x; t) dx = \int\limits_{N(v_1)} \left(\eta_{v_1}(x) \lim_{t\to 0} u_{v_2}(x; t) \right) dx.$$

Hence,

$$\lim_{t\to 0} H_0(v_1, v_2; t) = \frac{1}{\sqrt{\mu_{v_1}\mu_{v_2}}} \int\limits_{N(v_1)} \eta_{v_1}(x) \eta_{v_2}(x) dx.$$

If $v_1 \neq v_2$, the functions η_{v_1} and η_{v_2} have disjoint support, implying that $\lim_{t\to 0} H_0(v_1, v_2; t) = 0$. If $v_1 = v_2$, we get that

$$\lim_{t\to 0} H_0(v_1, v_1; t) = \frac{1}{\mu_{v_1}} \int\limits_{N(v_1)} \eta^2_{v_1}(x) dx = 1,$$

by assumption (c) regarding the function η_v. This proves assertion (i).

To prove (ii), consider two arbitrary and fixed vertices $v_1, v_2 \in VG$. Since the function $\frac{\partial^k}{\partial t^k} H_0(v_1, v_2; t)$ is right-continuous in $t \geq 0$, there exists $\delta = \delta(v_1, v_2, k)$ such that

$$\left| \frac{\partial^k}{\partial t^k} H_0(v_1, v_2; t) \right| \leq 1 + \left| \lim_{t\to 0} \left(\frac{\partial^k}{\partial t^k} H_0(v_1, v_2; t) \right) \right|,$$

for all $t \in (0, \delta)$. Let us fix such $\tilde{\delta} = \tilde{\delta}(v_1, v_2, k)$. To prove that $\left| \frac{\partial^k}{\partial t^k} H_0(v_1, v_2; t) \right|$ is bounded on $(0, \tilde{\delta})$ it suffices to show that $\left| \lim_{t\to 0} (\frac{\partial^k}{\partial t^k} H_0(v_1, v_2; t)) \right|$ is bounded. Let us take $k = 1$ first, to illustrate our approach.

From the definition (19) of H_0, the dominated convergence theorem implies that

$$\lim_{t\to 0} \frac{\partial}{\partial t} H_0(v_1, v_2; t) = \sqrt{\frac{\mu_{v_1}}{\mu_{v_2}}} \frac{1}{\mu_{v_1}} \int\limits_{N(v_1)} \lim_{t\to 0} \left(\frac{\partial}{\partial t} u_{v_2}(x; t) \right) \eta_{v_1}(x) dx.$$

Recall that $u_{v_2}(x; t)$ is a solution to the initial-value problem (20) and (21) with $v = v_2$. As such, the continuity of $u_{v_2}(x; t)$ and $\Delta_\Omega u_{v_2}(x; t)$ in the t-variable implies that

$$\begin{aligned} \lim_{t\to 0} \left(\frac{\partial}{\partial t} u_{v_2}(x; t) \right) &= \lim_{t\to 0} (-\Delta_\Omega u_{v_2}(x; t)) \\ &= -\Delta_\Omega u_{v_2}(x; 0) = -\Delta_\Omega \eta_{v_2}(x). \end{aligned}$$

Therefore,

$$\lim_{t\to 0}\frac{\partial}{\partial t}H_0(v_1,v_2;t) = \sqrt{\frac{\mu_{v_1}}{\mu_{v_2}}}\cdot\frac{1}{\mu_{v_1}}\int\limits_{N(v_1)}(-\Delta_\Omega\eta_{v_2}(x))\eta_{v_1}(x)dx.$$

As a result, we have that

$$\lim_{t\to 0}\frac{\partial}{\partial t}H_0(v_1,v_2;t) = 0 \quad \text{if } v_1 \neq v_2 \tag{24}$$

and

$$\lim_{t\to 0}\frac{\partial}{\partial t}H_0(v_1,v_1;t) = \frac{1}{\mu_{v_1}}\int\limits_{N(v_1)}(-\Delta_\Omega\eta_{v_1}(x))\eta_{v_1}(x)dx. \tag{25}$$

We now can apply the mean value theorem for integrals, which is justified because η_v is non-negative and $\Delta_\Omega\eta_{v_1}(x)$ is continuous. In doing so, we conclude that for some $x_1 \in N(v_1)$ we have the bounds

$$\lim_{t\to 0}\frac{\partial}{\partial t}H_0(v_1,v_1;t) \leq |\Delta_\Omega\eta_{v_1}(x_1)|\cdot\frac{1}{\mu_{v_1}}\int\limits_{N(v_1)}\eta_{v_1}(x)dx \leq |\Delta_\Omega\eta_{v_1}(x_1)|,$$

where the last inequality follows from (18). Therefore,

$$\left|\lim_{t\to 0}(\frac{\partial}{\partial t}H_0(v_1,v_2;t))\right| \leq |\Delta_\Omega\eta_{v_1}(x_1)|\cdot\delta_{v_1=v_2},$$

for some $x_1 \in N(v_1)$. For all $v \in VG$, the functions η_v are smooth. Let us define

$$C_k(v) := \sup_{x\in N(v)}\left|\Delta_\Omega^k\eta_v(x)\right|,$$

where Δ_Ω^k denotes the operator Δ_Ω applied k times. Then we have that

$$\left|\lim_{t\to 0}(\frac{\partial}{\partial t}H_0(v_1,v_2;t))\right| \leq C_1(v_1)\cdot\delta_{v_1=v_2}.$$

Consequently, we have that $\frac{\partial}{\partial t}H_0(v_1,v_2;t)$ is bounded by a constant which is independent of t for all $t \in (0,\tilde{\delta})$. The proof of (ii) in the case $k=1$ is now complete.

When $k>1$, we proceed in a similar manner. Namely, we write that

$$\lim_{t\to 0}\frac{\partial^k}{\partial t^k}H_0(v_1,v_2;t) = \sqrt{\frac{\mu_{v_1}}{\mu_{v_2}}}\frac{1}{\mu_{v_1}}\int\limits_{N(v_1)}\lim_{t\to 0}\left(\frac{\partial^k}{\partial t^k}u_{v_2}(x;t)\right)\eta_{v_1}(x)dx.$$

Since the functions η_v are C^∞,

$$\begin{aligned}\lim_{t\to 0}\left(\frac{\partial^k}{\partial t^k}u_{v_2}(x;t)\right) &= \lim_{t\to 0}\left((-1)^k\Delta_\Omega^k u_{v_2}(x;t)\right)\\ &= (-1)^k\Delta_\Omega^k u_{v_2}(x;0) = (-1)^k\Delta_\Omega^k\eta_{v_2}(x),\end{aligned}$$

and arguing as above, we get

$$\left|\lim_{t\to 0}(\frac{\partial^k}{\partial t^k}H_0(v_1,v_2;t))\right| \leq C_k(v_1)\cdot\delta_{v_1=v_2}.$$

Therefore $\frac{\partial^k}{\partial t^k}H_0(v_1,v_2;t)$ is bounded by a constant which is independent of t for all $t \in (0,\tilde{\delta})$.

For any fixed $\tilde{\delta} > 0$, the function $\frac{\partial^k}{\partial t^k}K(x,y;t)$ is uniformly bounded on the set $\Omega\times\Omega\times[\tilde{\delta},\infty]$, by a constant $C_{\tilde{\delta},k}$, see [Gr09]. Therefore, for all $v_1, v_2 \in VG$ and $t \geq \tilde{\delta}$,

$$\left|\frac{\partial^k}{\partial t^k}H_0(v_1,v_2;t)\right| \leq C_{\tilde{\delta},k}\frac{1}{\sqrt{\mu_{v_1}\mu_{v_2}}}\int\limits_{N(v_1)}\int\limits_{N(v_2)} \eta_{v_1}(x)\eta_{v_2}(y)\,dy\,dx \leq C_{\tilde{\delta},k}m(\Omega) \tag{26}$$

by (18). We have shown that $\frac{\partial^k}{\partial t^k}H_0(v_1,v_2;t)$ is bounded by a constant independent of t for all $t \in [\tilde{\delta},\infty)$, and the proof of the proposition is complete. □

From the above proposition it is evident that $H_0(v_1,v_2;t)$, defined by (19) is a parametrix of order zero for the heat kernel on G. This parametrix possesses continuous and bounded derivatives in t of any order (see (23)), hence, it is possible to further refine it and define a parametrix of higher order, by applying Proposition 6. For example, combining Proposition 6 with $n=1$, and equations (24) and (25) we deduce the following corollary.

Corollary 9. *With the notation as above, and for any $v_1, v_2 \in VG$, let*

$$u_1(v_1,v_2) = \begin{cases} d(v_1) - \frac{1}{\mu_{v_1}}\int\limits_{N(v_1)}(\Delta_\Omega\eta_{v_1}(x))\eta_{v_1}(x)dx, & \text{if } v_1 = v_2; \\ -w_{v_1v_2}, & \text{if } v_1 \sim v_2; \\ 0, & \text{otherwise,} \end{cases} \tag{27}$$

where $d(v_1) = \sum_{v\sim v_1} w_{vv_1}$ is the degree of the vertex v_1. Then

$$H_1(v_1,v_2;t) := H_0(v_1,v_2;t) - tu_1(v_1,v_2)$$

is a parametrix for the heat operator on G of order $k=1$.

Theorem 5 combined with the above corollary yields the following asymptotic formula relating the heat kernel on the graph G with the heat kernel of the "ambient space" Ω for small time t.

Corollary 10. *With the notation described in this section we have the following formula relating the heat kernel H_G on the graph G embedded in Ω, with the heat kernel K on Ω:*

$$H_G(v_1,v_2;t) = \frac{1}{\sqrt{\mu_{v_1}\mu_{v_2}}}\int\limits_{N(v_1)}\int\limits_{N(v_2)} K(x,y;t)\eta_{v_1}(x)\eta_{v_2}(y)dydx +$$
$$t\left[\delta_{v_1\sim v_2}w_{v_1v_2} - \delta_{v_1=v_2}d(v_1) + \frac{\delta_{v_1=v_2}}{\mu_{v_1}}\int\limits_{N(v_1)}(\Delta_\Omega\eta_{v_1}(x))\eta_{v_1}(x)dx\right] + O(t^2), \text{ as } t \to 0,$$

where the implied constant depends upon $v_1, v_2 \in VG$ and $\delta_{v_1\sim v_2} = 1$ if v_1 is adjacent to v_2 and $\delta_{v_1\sim v_2} = 0$, otherwise.

Remark 11. The normalization factor $\frac{1}{\sqrt{\mu_{v_1}\mu_{v_2}}}$ in the definition (19) was chosen so that

$$H_0(v_1,v_2;t) = H_0(v_2,v_1;t).$$

If one defines

$$\mathcal{H}_0(v_1, v_2; t) := \frac{1}{\mu_{v_1}} \int\limits_{N(v_1)} \int\limits_{N(v_2)} K(x, y; t)\eta_{v_1}(x)\eta_{v_2}(y)dydx., \tag{28}$$

it is easy to see that $\mathcal{H}_0(v_1, v_2; t)$ is also a parametrix of order zero for the heat kernel on G. The normalization in (28) can be justified by the fact that in the construction of the heat kernel on G the graph Laplacian acts only to the first variable and the formula (28) can be written as

$$\mathcal{H}_0(v_1, v_2; t) = \frac{1}{\mu_{v_1}} \int\limits_{N(v_1)} \eta_{v_1}(x)u_{v_2}(x; t)dx,$$

which can be veiwed as an "averaged by η_{v_1}" discretization; see Definition 4.1 on p. 689 of [BIK14]. The function $u_{v_2}(x; t)$ is a solution to the initial value problem (20) and (21).

5 Heat kernels for subgraphs

Let G be a finite or infinite subgraph of a finite or infinite weighted graph $\tilde{G}$ with the weight function $\tilde{w}_{xy}$ for vertices $x, y \in V\tilde{G}$. For us, a subgraph G of $\tilde{G}$ is obtained by using a subset VG of the vertices $V\tilde{G}$ defining the weight function w_{xy} for $x, y \in VG$ to be equal either to the same weight $\tilde{w}_{xy}$ on $\tilde{G}$ or set to zero. In the case when $\tilde{w}_{xy} \neq 0$ but $w_{xy} = 0$, we say that we have removed the edge connecting x and y in $\tilde{G}$. We define

$$\tilde{\mu}(x) = \sum_{y \in V\tilde{G}} \tilde{w}_{xy} \text{ and } \mu(x) = \sum_{y \in VG} w_{xy}. \tag{29}$$

When the graph $\tilde{G}$ is infinite, we assume that for all $x \in V\tilde{G}$, the function $\tilde{w}(x, \cdot)$ has finite support and that the quantity $\tilde{\mu}(x)$ is uniformly bounded for $x \in V\tilde{G}$. In this case, we say that $\tilde{G}$ has *bounded valence*. We further assume that $\tilde{G}$ is of bounded degree. Let ∂G denote the set of *boundary vertices* of the subgraph G in $\tilde{G}$. That is, ∂G consists of vertices $x \in VG$ such that $\mu(x) < \tilde{\mu}(x)$. We call $\mathrm{Int}(G) = VG \setminus \partial G$ the set of interior points of G.

Let $H_{\tilde{G}}$ denote the heat kernel for the graph $\tilde{G}$ with respect to the weighted graph Laplacian $\Delta_{\tilde{G}}$. Recall that for any function $f : V\tilde{G} \to \mathbb{C}$

$$\Delta_{\tilde{G}} f(x) = \sum_{y \in \tilde{G}} (f(x) - f(y))\tilde{w}_{xy}.$$

The Laplacian $\Delta_{\tilde{G}}$ is a non-negative and self-adjoint operator on the Hilbert space $L^2(V\tilde{G})$. Under our assumptios of finite valence and finite degree, the existence and uniqueness of the heat kernel follows from [DM06].

Let $L_{\tilde{G},v_1} = \Delta_{\tilde{G},v_1} + \partial_t$ be the heat operator on $\tilde{G}$ acting in the first variable, and let $L_{G,v_1} = \Delta_{G,v_1} + \partial_t$ be the heat operator on G. Define

$$H(v_1, v_2; t) := H_{\tilde{G}}(v_1, v_2; t) \quad \text{for } v_1, v_2 \in VG \text{ and } t \geq 0.$$

In other words, H is the restriction of the heat kernel from $\tilde{G}$ to G. Clearly, if $v_1 \in \mathrm{Int}(G)$ we have $L_{G,v_1} H(v_1, v_2; t) = 0$, but if $v_1 \in \partial G$ then

$$L_{G,v_1} H(v_1, v_2; t) = - \sum_{v \in A_{\tilde{G},G}(v_1)} \left(H(v_1, v_2; t) - H(v, v_2; t)\right) w_{v_1 v}, \tag{30}$$

where

$$A_{\tilde{G},G}(v_1) = \{v \in V\tilde{G} \setminus VG : v \text{ is adjacent to } v_1 \text{ in } \tilde{G}\} \cup \{v \in VG : \tilde{w}_{vv_1} \neq 0 \text{ but } w_{vv_1} = 0\}.$$

The set $A_{\tilde{G},G}(v_1)$ is not empty for $v_1 \in \partial G$, so one cannot expect that the difference (30) to vanish so H is certainly not the heat kernel on G. However, we show in the following proposition that $H(v_1, v_2; t)$ is a parametrix of order zero for the heat kernel on G.

Proposition 12. *Assume the notation as above.*

(i) For all $v_1, v_2 \in VG$, we have that

$$\lim_{t \to 0} H(v_1, v_2; t) = \begin{cases} 1 & \text{if } v_1 = v_2 \\ 0 & \text{if } v_1 \neq v_2. \end{cases} \tag{31}$$

(ii) For $v_1, v_2 \in VG$, there is a constant $C(v_1, v_2)$ such that for all $t > 0$, we have that

$$\left| \frac{\partial}{\partial t} H(v_1, v_2; t) \right| \leq C(v_1, v_2). \tag{32}$$

Proof. Part (i) follows trivially from the fact that $H(v_1, v_2; t)$ is the restriction of the heat kernel on $\tilde{G}$, so it remains to prove part (ii).

Since $H(v_1, v_2; t) = H_{\tilde{G}}(v_1, v_2; t)$ for $v_1, v_2 \in VG$,

$$\frac{\partial}{\partial t} H(v_1, v_2; t) = -\Delta_{\tilde{G}, v_1} H(v_1, v_2; t) = \sum_{y \in VG} H(y, v_2; t) \tilde{w}_{v_1 y} - H(v_1, v_2; t) \mu(v_1).$$

Both $\tilde{w}$ and μ are bounded, so in order to prove (32), it suffices to show that $H(v_1, v_2; t)$ is bounded as a function of t for fixed v_1, v_2 by some constant, which may depend upon v_1 and v_2. We could not find a convenient reference for this fact so we provide a short proof for the sake of completeness.

The Dirac property (31) implies that $H(v_1, v_2; t)$ is bounded by an explicit constant, such as 2, when viewed as a function of t for $t \in [0, \eta)$ for some $\eta > 0$. It remains to prove boundedness for $t \in [\eta, \infty)$. In the case when $V\tilde{G}$ is finite, we can use the spectral expansion of the heat kernel as a sum over eigenfunctions ψ_j of the Laplacian $\Delta_{\tilde{G}}$ and the Cauchy-Schwartz inequality to deduce that for $t \geq \eta$ one has

$$\begin{aligned} |H(v_1, v_2; t)| &\leq \left(\sum_j e^{-\lambda_j t} |\psi_j(v_1)|^2 \right)^{1/2} \left(\sum_j e^{-\lambda_j t} |\psi_j(v_2)|^2 \right)^{1/2} \\ &\leq \left(H(v_1, v_1; \eta) H(v_2, v_2; \eta) \right)^{1/2}. \end{aligned} \tag{33}$$

Note that the fact that the eigenvalues λ_j are nonnegative implies that each $e^{-\lambda_j t}$ above is nonincreasing on $t > 0$. If $V\tilde{G}$ is infinite, one re-writes the sums in (33) as integrals over the appropriate spectral measures, and one gets that $H(v_1, v_2; t)$ is bounded for $t \geq \eta$ by $(H(v_1, v_1; \eta) H(v_2, v_2; \eta))^{1/2}$. This completes the proof of the claim. □

If the graph G is a *finite* subgraph of $\tilde{G}$, Theorem 5 applies to deduce the heat kernel on G from the parametrix $H(v_1, v_2; t)$. However, the parametrix construction of the heat kernel on infinite subgraph of a finite valence infinite graph $\tilde{G}$ can also be carried out, under the assumption that the boundary ∂G of G is finite. The precise result is the following proposition.

Proposition 13. *Let G be an infinite subgraph of a finite valence, bounded degree graph $\tilde{G}$ such that boundary ∂G is finite. Let $\tilde{H}(v_1, v_2; t)$ denote the heat kernel on $\tilde{G}$. Then the series*

$$\sum_{\ell=1}^{\infty}(-1)^{\ell}(L_{G,v_1}\tilde{H})^{*\ell}(v_1, v_2; t) \tag{34}$$

converges absolutely and uniformly on any compact subset of $VG \times VG \times [0, \infty)$ and defines a function $\tilde{F}(v_1, v_2; t)$ on $VG \times VG \times [0, \infty)$. Furthermore, the heat kernel $H_G(v_1, v_2; t)$ on G is given by

$$H_G(v_1, v_2; t) := \tilde{H}(v_1, v_2; t) + (\tilde{H} * \tilde{F})(v_1, v_2; t).$$

Proof. We start by observing that the function $L_{G,v_1}\tilde{H}(v_1, v_2; t)$ when viewed as a function of the first variable is supported on the finite set ∂G. Moreover, the heat kernel $\tilde{H}(v_1, v_2; t)$ is bounded. Hence, there exists a constant C depending on the finite subset ∂G of G and the valence of G so that

$$\begin{aligned}(L_{G,v_1}\tilde{H} * L_{G,v_1}\tilde{H})(v_1, v_2; t) &= \sum_{v\in\partial G}\int_0^t L_{G,v_1}\tilde{H}(v_1, v; t-\tau)L_{G,v_1}\tilde{H}(v, v_2; \tau)d\tau \\ &\leq |\partial G| \cdot Ct,\end{aligned}$$

for all $(v_1, v_2) \in \partial G \times VG$ and all $t \geq 0$, where $|\partial G|$ denotes the number of elements in ∂G. By arguing analogously as in the proof of Lemma 3, we conclude that the series (34) converges absolutely and uniformly on any compact subset of $VG \times VG \times [0, \infty)$. The Dirac property $\lim_{t\to 0}\tilde{H}(v_1, v_2; t) = \delta_{v_1=v_2}$ when combined with the finiteness of support of $L_{G,v_1}\tilde{H}(v_1, v_2; t)$ is sufficient to conclude that Lemma 4 also holds with $H = \tilde{H}$. The method of the proof of Theorem 5 then applies to show that $H_G(v_1, v_2; t)$ is the heat kernel on G. □

6 A subgraph of the complete graph on N vertices

In this section we will develop explicitly our results in the setting of a subgraph of the complete graph on N vertices. Throughout this section we will employ some of the same considerations as in [LNY21], namely in the explicit computation of the graph convolution. In doing so, we will show the relationship between our Theorem 5 and Theorem 3.3 of [LNY21].

Let K_N denote the complete graph K_N on N vertices. Let us label the vertices with the integers $1, 2, \cdots, N$ and define the weights to be $\tilde{w}_{xy} = 1$ for all $x \neq y$. In the notation of the previous section, K_N plays the role of $\tilde{G}$. The heat kernel on K_N is well known. Indeed, if we set $H_{\tilde{G}} := H_{K_N}$, then we have that

$$H_{\tilde{G}}(x, y; t) := \begin{cases} \frac{1}{N} + \left(1 - \frac{1}{N}\right)e^{-Nt}, & \text{for } x = y \\ \frac{1}{N} - \frac{1}{N}e^{-Nt}, & \text{otherwise.}\end{cases} \tag{35}$$

Let G be any subgraph of K_N. Without loss of generality, we assume that G has N vertices, and take $H_{\tilde{G}}$ as a parametrix for the heat kernel H_G on G. In order to compare our results with those from [LNY21], we will borrow and adapt some notation from [LNY21].

For any vertex $x \in VG$, let d_x^G be the degree of x in G and set $d_x^c = (N-1) - d_v^G$. For two vertices $x \in VG$ and $y \in VK_N$, let us write $x \sim_c y$ if $x \neq y$ and x and y are not connected in G. Define the combinatorial Laplacian on the complement of G in K_N by

$$\Delta^c f(x) = \sum_{y\sim_c x}(f(x) - f(y)) \tag{36}$$

From (30) we have that

$$L_1 H_{\tilde{G}}(x,y;t) = -\sum_{z\sim_c x} \left(H_{\tilde{G}}(x,y;t) - H_{\tilde{G}}(z,y;t) \right),$$

for all $x, y \in VG$ and any $t > 0$. Note that we have shortened the notation by lettng L_1 denote the heat operator of G acting on the first vertex variable x. From the expression (35) for the heat kernel $H_{\tilde{G}}$, we immediately have for $x, y \in VG$ that

$$L_1 H_{\tilde{G}}(x,y;t) = \begin{cases} -e^{-Nt} d_x^c, & \text{if } x = y : \\ e^{-Nt}, & \text{if } x \sim_c y; \\ 0, & \text{otherwise.} \end{cases} \tag{37}$$

In the notation of formula (3.4) from [LNY21],

$$L_1 H_{\tilde{G}}(x,y;t) = -e^{-Nt} u_y^c(x). \tag{38}$$

(We write u_y^c for $u_y^{G^c}$ in [LNY21].)

In Section 3 of [LNY21] the authors define an operator T which acts on functions $F : VG \times VG \times \mathbb{R}_{>0}$ by

$$\begin{aligned} TF(x,y;t) &= \int_0^t e^{-N(t-s)} \Delta_x^c F(x,y;s)\, ds \\ &= \int_0^t e^{-N(t-s)} (d_x^c F(x,y;s) - \sum_{\substack{v\in VG \\ v\sim_c x}} F(v,y;s))\, ds. \end{aligned} \tag{39}$$

In other words

$$TF(x,y;t) = -(L_1 H_{\tilde{G}} * F)(x,y;t).$$

This explains the connection between our Theorem 5:

$$H_G(x,y;t) = H_{\tilde{G}}(x,y;t) + \sum_{l=1}^{\infty} (-1)^l ((L_1 H_{\tilde{G}})^{*l} * H_{\tilde{G}})(x,y;t)$$

and equation (3.3) of [LNY21]:

$$H_G(x,y;t) = \sum_{l=0}^{\infty} T^l H_{\tilde{G}}(x,y;t).$$

Theorem 3.3 of [LNY21] goes further to show that

$$H_G(x,y;t) = H_{\tilde{G}}(x,y;t) + te^{-Nt} u_y^c(x) + \sum_{\ell=2}^{\infty} (-1)^{\ell-1} \frac{t^\ell}{\ell!} e^{-Nt} \left(\Delta_x^c\right)^{\ell-1} u_y^c(x).$$

We can give a slightly different expression for $H_G(x,y;t)$ using matrix notation. Since G is undirected we have $u_x^c(y) = u_y^c(x)$ for all $x, y \in VG$. Let B denote the $N \times N$ symmetric matrix with elements $b_{xy} = u_x^c(y) = u_y^c(x)$. Then starting with (38), it is easy to inductively show that

$$\left(H_{\tilde{G}} * (L_1 H_{\tilde{G}})^{*\ell} \right)(x,y;t) = (-1)^\ell \frac{t^\ell}{\ell!} e^{-Nt} B^\ell(x,y),$$

Therefore,

$$H_G(x,y;t) = H_{\tilde{G}}(x,y;t) + e^{-Nt} \sum_{\ell=1}^{\infty} \frac{t^\ell}{\ell!} B^\ell(x,y).$$

Let us highlight the example when G is a subgraph of K_N obtained by deleting one edge from K_N.

Example 14. Let $G_{1,2}$ be the graph that results from deleting the edge between 1 and 2 in K_N. In this case, $B = (b_{ij})_{N\times N}$ with $b_{11} = b_{22} = 1$; $b_{12} = b_{21} = -1$ and all other entries of B are zeros. Inductively, it is straightforward to show for any $\ell \geq 1$ we have that

$$B^\ell(x, y) = \begin{cases} 2^{\ell-1}, & \text{if } x = y \in \{1, 2\}, \\ -2^{\ell-1}, & \text{if } x, y \in \{1, 2\},\ x \neq y, \\ 0, & \text{otherwise.} \end{cases}$$

Therefore

$$H_G(x, y; t) = H_{\tilde{G}}(x, y; t)$$

except when $x, y \in \{1, 2\}$, in which case we have that

$$\begin{aligned} H_G(x, x; t) &= H_{\tilde{G}}(x, x; t) + e^{-Nt} \sum_{\ell=1}^{\infty} 2^{\ell-1} \frac{t^\ell}{\ell!} \\ &= H_{\tilde{G}}(x, x; t) + e^{-Nt}(e^{2t} - 1)/2 \end{aligned}$$

and

$$\begin{aligned} H_G(x, y; t) &= H_{\tilde{G}}(x, y; t) - e^{-Nt} \sum_{\ell=1}^{\infty} 2^{\ell-1} \frac{t^\ell}{\ell!} \\ &= H_{\tilde{G}}(x, y; t) - e^{-Nt}(e^{2t} - 1)/2 \quad \text{for } x \neq y. \end{aligned}$$

These computations show very explicitly and simply the effect on the heat kernel from deleting an edge in the complete graph. Specifically, one sees the change by a negative number in $K_G(1, 2; t)$ reflecting the disconnect between the vertices 1 and 2.

7 Heat kernel on a discrete half-line

The following example illustrates the construction of the heat kernel on an infinite subgraph with finite boundary.

Example 15. Let G be a discrete half-line beginning with 0. More precisely, G is the graph with vertices consisting of non-negative integers such that each positive integer j is connected only to its neighbors $j + 1$ and $j - 1$, while 0 is connected only to 1. Then G is an infinite subgraph of $\tilde{G} = \mathbb{Z}$ with the finite boundary $\partial G = \{0\}$. Therefore Proposition 13 applies to give an expression for the heat kernel on G by using the heat kernel $H(v, w; t)$ on $\mathbb{Z}$ as a parametrix. Let us carry out these calculations in detail.

Recall that $H(v, w; t) = e^{-2t} I_{v-w}(2t)$; see [KN06]. The heat operator of G acts on the $\mathbb{Z}$ heat kernel H as

$$L_{G,v}H(v, w; t) = \begin{cases} e^{-2t}(I_{w+1}(2t) - I_w(2t)), & \text{if } v = 0; \\ 0, & \text{otherwise.} \end{cases}$$

Hence, the heat kernel on the discrete half-line G is given by

$$H_G(v, w; t) = e^{-2t} I_{|v-w|}(2t) + \sum_{\ell=1}^{\infty} (-1)^\ell \left(H * (L_{G,v}H)^{*\ell} \right)(v, w; t). \tag{40}$$

We will now compute explicitly the convolution series on the right-hand side of (40). We start by observing that

$$\begin{aligned}(H*(L_{G,v}H))(v,w;t) &= \int_0^t H(v,0;t-\tau)L_{G,v}H(0,w;\tau)d\tau \\ &= \frac{1}{2}e^{-2t}\int_0^{2t} I_v(2t-u)\left(I_{w+1}(u)-I_w(u)\right)du. \qquad (41)\end{aligned}$$

Next, we derive a formula for the classical convolution of I-Bessel functions. Let m,n be non-negative integers. For $x\geq 0$ we start with formula (1) on page 379 of [Wa66]. In the notation from [Wa66] we take $\mu=m$ and $\nu=n$ and complex z to get that

$$z\int_0^{\pi/2} J_m(z\cos^2\phi)J_n(z\sin^2\phi)\sin\phi\cos\phi d\phi = \sum_{k=0}^{\infty}(-1)^k J_{m+n+2k+1}(z),$$

where J stands for the classical J-Bessel function of the first kind. By replacing z with iz and applying the identity $J_n(iz)=i^n I_n(z)$ (see [GR07], formula 8.406.3), the above equation becomes

$$z\int_0^{\pi/2} I_m(z\cos^2\phi)I_n(z\sin^2\phi)\sin\phi\cos\phi d\phi = \sum_{k=0}^{\infty} I_{m+n+2k+1}(z).$$

The change of variables $t=z\sin^2\phi$ gives that

$$\int_0^x I_n(t)I_m(x-t)dt = 2\sum_{k=0}^{\infty} I_{m+n+2k+1}(x). \qquad (42)$$

Combining (41) and (42) we arrive at

$$(H*(L_{G,v}H))(v,w;t) = e^{-2t}\sum_{k=1}^{\infty}(-1)^k I_{v+w+k}(2t).$$

Applying the identity (42) once again, it is immediate to see that

$$\begin{aligned}\left(H*(L_{G,v}H)^{*2}\right)(v,w;t) &= \left((H*(L_{G,v}H))*(L_{G,v}H)\right)(v,w;t) \\ &= e^{-2t}\sum_{(k_1,k_2)\in\mathbb{N}^2}(-1)^{k_1+k_2}I_{v+w+k_1+k_2}(2t).\end{aligned}$$

A simple inductive argument yields that, for any $\ell\geq 1$ the following identity holds true

$$\left(H*(L_{G,v}H)^{*\ell}\right)(v,w;t) = e^{-2t}\sum_{(k_1,\ldots k_\ell)\in\mathbb{N}^\ell}(-1)^{k_1+\ldots k_\ell}I_{v+w+k_1+\ldots k_\ell}(2t).$$

Therefore,

$$\sum_{\ell=1}^{\infty}(-1)^\ell\left(H*(L_{G,v}H)^{*\ell}\right)(v,w;t) = e^{-2t}\sum_{n=1}^{\infty}a(n)I_{v+w+n}(2t),$$

where $a(1) = 1$ and

$$a(n) = (-1)^n \sum_{\ell=1}^{n} (-1)^\ell |S(n,\ell)|, \quad \text{for} \quad n \geq 2,$$

where $|S(n,\ell)|$ is the cardinality of the set $S(n,\ell) = \{(k_1, \dots k_\ell) \in \mathbb{N}^\ell : k_1 + \dots k_\ell = n\}$. Actually, $|S(n,\ell)|$ is the number of ordered partitions of $n \geq 2$ into $\ell \geq 1$ parts and it equals $\binom{n-1}{\ell-1}$, hence

$$a(n) = (-1)^n \sum_{\ell=1}^{n} (-1)^\ell \binom{n-1}{\ell-1} = 0, \quad \text{for} \quad n \geq 2.$$

This proves that

$$\sum_{\ell=1}^{\infty} (-1)^\ell \left(H * (L_{G,v} H)^{*\ell} \right)(v, w; t) = e^{-2t} I_{v+w+1}(2t),$$

hence the heat kernel on a discrete half-line is given by

$$H_G(v, w; t) = e^{-2t} \left(I_{|v-w|}(2t) + I_{v+w+1}(2t) \right).$$

8 The Dirichlet heat kernel on a graph

Let G be a subgraph of a (possibly infinite) graph $\tilde{G}$ of finite and bounded valence. As above, we denote the set of boundary points of G by ∂G. We denote the set of interior points of G by $\mathrm{Int}(G) = VG \setminus \partial G$. Similarly, we may view the graph with the vertex set $VG \setminus \partial G$ and edges between the elements of the vertex set inherited from G to be a subgraph of G. The boundary of this subgraph will be denoted by $\partial(G \setminus \partial G)$.

We define the Dirichlet heat kernel $H_{D,G}(v_1, v_2; t) : VG \times VG \times [0, \infty)$ on G with boundary ∂G in analogy to the Dirichlet problem on a manifold with the boundary, or on a regular domain; see, for example Chapter VII of [Ch84]. Specifically, we define $H_{D,G}(v_1, v_2; t)$ to be the solution to the differential equation

$$L_{G,v_1} H_{D,G}(v_1, v_2; t) := \left(\Delta_{G,v_1} + \frac{\partial}{\partial t} \right) H_{D,G}(v_1, v_2; t) = 0, \text{ if } v_1 \in G \setminus \partial G$$

with the property that

$$\lim_{t \to 0} H_{D,G}(v_1, v_2, t) = \delta_{v_1 = v_2} \quad \text{for } v_1 \in G \setminus \partial G$$

together with the Dirichlet boundary condition

$$H_{D,G}(v_1, v_2; t) = 0 \quad \text{for all } v_2 \in G \text{ and } t \geq 0 \text{ whenever } v_1 \in \partial G.$$

The existence and uniqueness of the Dirichlet heat kernel readily follows from results in [Hu12]. The Dirichlet heat kernel in the setting of a discrete interval was constructed from the heat kernel on $\mathbb{Z}$ in [Do12] using a symmetry based method of images.

Proposition 16. *Let $\tilde{G}$ be a finite or infinite graph with bounded valence. Let G be a subgraph of $\tilde{G}$ such that boundaries ∂G and $\partial(G \setminus \partial G)$ are finite. Let $\tilde{H}(v_1, v_2; t)$ denote the heat kernel on $\tilde{G}$. For $(v_1, v_2; t) \in VG \times VG \times [0, \infty)$ define the function*

$$H_0(v_1, v_2; t) := \begin{cases} \tilde{H}(v_1, v_2; t), & \text{for } v_1 \in VG \setminus \partial G, v_2 \in VG, t \geq 0 \\ 0, & \text{otherwise.} \end{cases}$$

Then the series

$$\sum_{\ell=1}^{\infty}(-1)^{\ell}(L_{G,v_1}H_0)^{*\ell}(v_1,v_2;t) \tag{43}$$

converges absolutely and uniformly on any compact subset of $VG\times VG\times[0,\infty)$. *Furthermore, the Dirichlet heat kernel* $H_{D,G}(v_1,v_2;t)$ *on* G *is given by*

$$H_{D,G}(v_1,v_2;t):=H_0(v_1,v_2;t)+(H_0*F)(v_1,v_2;t). \tag{44}$$

Proof. First, we note that our assumptions on $\tilde{G}$ ensure existence and uniqueness of $\tilde{H}$; see for example [DM06]). Hence, the function H_0 is well defined. Let $L_{\tilde{G},v_1}$ denote the heat operator on $\tilde{G}$. Then it is immediate that for all vertices $v_1\in VG\setminus(\partial G\cup\partial(G\setminus\partial G))$, all vertices $v_2\in VG$ and any $t\geq 0$ one has that

$$L_{\tilde{G},v_1}H_0(v_1,v_2;t)=L_{G,v_1}\tilde{H}(v_1,v_2;t)=0.$$

In particular, this shows that $L_{G,v_1}H_0(v_1,v_2;t)$ is supported on $(\partial G\cup\partial(G\setminus\partial G))\times VG\times[0,\infty)$. Therefore, for all $\ell\geq 1$, the convolution $(L_{G,v_1}H_0)^{*\ell}(v_1,v_2;t)$ is supported on the set $(\partial G\cup\partial(G\setminus\partial G))\times VG\times[0,\infty)$.

Choose an arbitrary, but fixed finite subset A of VG. We now will prove for any $T>0$ the convergence of the series (43) on the set $(\partial G\cup\partial(G\setminus\partial G))\times A\times[0,\infty)$, and that the convergence is absolute and uniform on the set.

From Proposition 12, the functions $H_0(v_1,v_2;t)$ and $\frac{\partial}{\partial t}H_0(v_1,v_2;t)$ are uniformly bounded in t. Denote an upper bound the two functions by $C(v_1,v_2)$. Therefore, for every finite subset A of VG the function $L_{G,v_1}H_0(v_1,v_2;t)$ is bounded by a certain constant $C(A)$ which depends only on the graph G and the set A, and can be chosen to be a constant depending on the graph and multiplied by $\max_{v_1\in(\partial G\cup\partial(G\setminus\partial G)),v_2\in A}\{C(v_1,v_2)\}$.

Let C denote the cardinality of the set $\partial G\cup\partial(G\setminus\partial G)$. Then

$$\begin{aligned}(L_{G,v_1}H_0*L_{G,v_1}H_0)(v_1,v_2;t)&=\sum_{v\in\partial G\cup\partial(G\setminus\partial G)}\int_0^t L_{G,v_1}H_0(v_1,v;t-\tau)L_{G,v_1}H_0(v,v_2;\tau)d\tau\\&=O\left(C\cdot C(A)t\right),\end{aligned}$$

where the implied constant depends only upon G. By proceeding as in the proof of Lemma 3, we deduce that

$$(L_{G,v_1}H_0)^{*\ell}(v_1,v_2;t)=O\left(C\cdot\frac{(C\cdot C(A)t)^{\ell-1}}{(\ell-1)!}\right),$$

where as before the implied constant depends only upon G. With these bounds, we have proved the absolute and uniform convergence of the series (43) on the set $(\partial G\cup\partial(G\setminus\partial G))\times A\times[0,\infty)$.

It is left to prove that the right-hand side of (44) is equal to the Dirichlet heat kernel $H_{D,G}(v_1,v_2;t)$ on G. For $v_1\in\partial G$, $v_2\in G$ and all $t\geq 0$, and by the definition of H_0 and convolution, it is immediate that $H_{D,G}(v_1,v_2;t)=0$. What remains is to prove that $L_{G,v_1}H_0(v_1,v_2;t)=0$ for all $v_1\in VG\setminus\partial G$, $v_2\in G$ and all $t\geq 0$.

When $v_1\in VG\setminus\partial G$, $H_0(v_1,v_2;t)=\tilde{H}(v_1,v_2;t)$. Hence, by reasoning as in the proof of Lemma 4, and by using the Dirac property of $\tilde{H}$ we get that

$$L_{G,v_1}(H_0*F)(v_1,v_2;t)=F(v_1,v_2;t)+((L_{G,v_1}H_0)*F)(v_1,v_2;t).$$

The absolute and uniform convergence of the series (43) suffices to deduce that $L_{G,v_1}H_0(v_1,v_2;t)=0$ for all $v_1\in VG\setminus\partial G$, $v_2\in G$ and all $t\geq 0$, as in the proof of Theorem 5. □

As an example, let us compute the fundamental solution to the Dirichlet problem on the discrete half-line $\{0, 1, 2, \ldots\}$ when starting with the heat kernel on the graph $\mathbb{Z}$.

Example 17. With the notation from Example 15, let G be the discrete half-line $\{0, 1, 2, \ldots\}$ when viewed as a subgraph of $\mathbb{Z}$. Let us set

$$H_0(x,y;t) := \begin{cases} e^{-2t} I_{|x-y|}(2t), & \text{for } x, y \in \mathbb{Z}, x \geq 1, y \geq 0 \\ 0, & \text{if } x = 0. \end{cases}$$

Then the Dirichlet heat kernel on G is given by Proposition 16. In order to compute it explicitly, one first notices that

$$L_{G,x} H_0(x,y;t) = \begin{cases} 0, & \text{when } x \geq 2; \\ e^{-2t} I_y(2t), & \text{when } x = 1 \\ -e^{-2t} I_{|y-1|}(2t), & \text{when } x = 0. \end{cases}$$

Let

$$F(x,y;t) := \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{G,x} H_0)^{*\ell}(x,y;t), \quad x, y = 0, 1, 2, \ldots; \quad t \geq 0.$$

When viewed as a function of the first variable x, $L_{G,x} H_0(x,y;t)$ is supported on the set $\{0, 1\}$. Then, $F(x,y;t)$ as a function of x is also supported on the set $\{0, 1\}$. Therefore, we need to find an expression for F when $x = 0$ and $x = 1$.

Case 1. When $x = 0$. First, we compute $(L_{G,x} H_0)^{*\ell}(0,y;t)$ for $\ell \geq 2$. When $y \geq 1$ we have that

$$(L_{G,x} H_0)^{*2}(0,y;t) = e^{-2t} \int_0^t (I_1(2(t-\tau)) I_{|y-1|}(2\tau) - I_0(2(t-\tau)) I_y(2\tau)) d\tau = 0$$

while

$$(L_{G,x} H_0)^{*2}(0,0;t) = -e^{-2t} I_1(2t) = L_{G,x} H_0(0,0;t).$$

Since $(L_{G,x} H_0)^{*2}(0,1;t) = 0$, we can now deduce that

$$(L_{G,x} H_0)^{*2\ell}(0,0;t) = (L_{G,x} H_0)^{*(2\ell-1)} H_0(0,0;t) \quad \text{for all } \ell \geq 1.$$

It is somewhat straightforward to show that $(L_{G,x} H_0)^{*2\ell}(0,y;t) = 0$ for all $y \neq 0$. Also, we have that

$$(L_{G,x} H_0)^{*(2\ell+1)}(0,y;t) = \frac{(-1)^{\ell+1} e^{-2t}}{2^{\ell}} ((I_1)^{*\ell} * I_{(y-1)})(2t), \quad \text{for } y \geq 1.$$

Note that the symbol $*$ in the above display is used for two types of convolution: the graph convolution on the left-hand side and the classical convolution of two functions on the right-hand side. We will continue using this notation, as it is clear from the context which type of convolution is used.

With all this, we can conclude that $F(0,0;t) \equiv 0$ for all $t \geq 0$ and

$$F(0,y;t) = \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell} e^{-2t}}{2^{\ell}} ((I_1)^{*\ell} * I_{|y-1|})(2t) \quad \text{for } y \geq 1,$$

where we interpret a 0-fold convolution to act as the identity operator:

$$((I_l)^{*0} * f)(t) = f(t) \text{ for all } f : (0, \infty) \to \mathbb{R}.$$

Case 2. $x = 1$. We shall compute $(L_{G,x}H_0)^{*\ell}(1, y; t)$ for $\ell \geq 2$. When $\ell = 2$ we get that

$$(L_{G,x}H_0)^{*2}(1, y; t) = e^{-2t} \int_0^t (I_1(2(t-\tau))I_y(2\tau) - I_0(2(t-\tau))I_{|y-1|}(2\tau))d\tau$$
$$= \begin{cases} 0, & \text{for } y = 0; \\ -e^{-2t} I_y(2t), & \text{for } y \geq 1. \end{cases}$$

Analogous calculations as in Case 1 give that

$$F(1, y; t) = \begin{cases} -2 \sum_{\ell=0}^{\infty} \frac{(-1)^\ell e^{-2t}}{2^\ell} ((I_1)^{*\ell} * I_y)(2t), & \text{for } y \geq 1; \\ - \sum_{\ell=0}^{\infty} \frac{(-1)^\ell e^{-2t}}{2^\ell} ((I_1)^{*\ell} * I_0)(2t)), & \text{for } y = 0. \end{cases}$$

We now can compute the convolution of H_0 and F in closed form. First, notice that the convolution of I_m and I_n depends only on the sum of m and n, and that it is commutative operation. Therefore, for $x, y \geq 1$ and $t \geq 0$ we have

$$\left(I_x * \left[(I_1)^{*\ell} * I_{y-1}\right]\right)(2t) = \left(I_{x-1} * \left[(I_1)^{*\ell} * I_y\right]\right)(2t) = \left[(I_1)^{*\ell} * (I_{x-1} * I_y)\right](2t).$$

The convolution series over ℓ converges absolutely and uniformly over compact subsets of $VG \times VG \times [0, \infty)$. With this, we get a closed formula for $H_0 * F(x, y; t)$. Specifically, for all $x \geq 1$, $y \geq 0$ and $t \geq 0$, we have that

$$H_0 * F(x, y; t) = e^{-2t} \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell+1} e^{-2t}}{2^{\ell+1}} \left((I_1)^{*\ell} * (I_{x-1} * I_y)\right)(2t).$$

Therefore, the Dirichlet heat kernel on the half-line $\{0, 1, 2, \ldots\}$ is given for $t \geq 0$ by

$$H_{D,G}(x, y; t) = e^{-2t} \begin{cases} I_{|x-y|}(2t) + \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell+1} e^{-2t}}{2^{\ell+1}} \left((I_1)^{*\ell} * (I_{x-1} * I_y)\right)(2t), & \text{for } x \geq 1, y \geq 0 \\ 0, & \text{if } x = 0. \end{cases}$$

On the other hand, it is easy to check directly that for all $x, y \geq 0$ and $t \geq 0$ the Dirichlet heat kernel on the half-line G can be expressed as

$$H_{D,G}(x, y; t) = e^{-2t}(I_{x-y}(2t) - I_{x+y}(2t)).$$

The uniqueness of the Dirichlet heat kernel immediately implies the identity that

$$I_{x+y}(t) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{2^{\ell+1}} \left((I_1)^{*\ell} * (I_{x-1} * I_y)\right)(t)$$

for all integers $x \geq 1$ and $y \geq 0$. From this expression, we will point out the two interesting special cases that

$$I_1(t) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{2^{\ell+1}} \left((I_1)^{*\ell} * (I_0)^{*2}\right)(t)$$

and

$$I_2(t) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{2^{\ell+1}} \left((I_1)^{*(\ell+1)} * I_0\right)(t).$$

Disclosures, Declarations, Data transparency

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