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The heat kernel on a finite graph in different time-scales

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Abstract: Let G be a finite, weighted graph, and let $\mathbb{T}$ be a time-scale with a fixed point t_0 such that $\sup \mathbb{T} = \infty$. In this paper, we construct the heat kernel on G in time-scale $\mathbb{T}$ in terms of a certain convolution series involving the heat operator acting on a parametrix, which is a fairly general function depending on the vertex set of G and the time variable $t \in \mathbb{T}$. We develop some applications by choosing different parametrices and various time-scales. The results we obtain here extend, in part, aspects of the recent articles in that the time-scale considered in this paper is arbitrary.

Key words: Heat kernel, finite graph, time-scales

1. Introduction

The heat equation characterizes the diffusion process within both discrete and continuous settings, often governed by specified boundary conditions. Its fundamental solution, the heat kernel, underpins extensive research within mathematical biology [5, 6, 9, 16, 27], computational mathematics [21], and stochastic processes [12, 22]. Given the diversity of these processes, a natural inquiry arises regarding the behavior of diffusive phenomena within hybrid systems, by which we mean systems that encompass both continuous and discrete aspects. To formalize the description of such phenomena in hybrid systems, we turn to time-scale calculus. Time-scales offer a unifying framework to generalize results across continuous and discrete domains, a pursuit of increasing interest from different mathematical disciplines and applications such as finance, biology, and physics, to name a few. This unification bridges difference equations and differential equations, thus showing the significance of the study of hybrid systems.

In this paper, we extend the work presented in [11] and construct the heat kernel on finite graphs for different time-scales. The extension we prove is far from being straightforward, mainly due to subtle nature of the shift in the setting of time-scales which is used to define the graph convolution. In this context, one begins with a parametrix which is a reasonably general approximation of the heat kernel and that depends solely on small time asymptotic behavior. The parametrix then undergoes an iterative refinement process which yields progressively more precise approximations of the heat kernel. Ultimately, the heat kernel is expressed as an infinite series involving the parametrix and a convolution series derived from the parametrix. Additionally, we will prove an extension to varying time-scales of the results from [23] which explicitly computes the heat kernel of a subgraph of the complete graph on $N > 1$ vertices. Since all finite graphs, indeed, are subgraphs of some

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complete graph, this computation yields a new evaluation of the heat kernel on any finite graph associated to any time-scale $\mathbb{T}$ such that $\sup\mathbb{T} = \infty$.

Let us now discuss some technical details. We begin by considering $\mathbb{T}$ as an arbitrary time-scale, which is a closed subset of the real numbers $\mathbb{R}$. Additionally, we assume the presence of a fixed point (the so-called base point) t_0 in $\mathbb{T}$, conventionally set to 0 yet capable of assuming other values within $\mathbb{T}$. For any $t \in \mathbb{T}$, let $\sigma(t) := \inf\{s \in \mathbb{T} : s > t\}$. The function $\sigma(t)$ is called the forward operator. While the graininess function $\mu : \mathbb{T} \to [0, \infty)$ is defined by $\mu(t) := \sigma(t) - t$.

Throughout this paper, unless otherwise stated, we assume the time-scale $\mathbb{T}$ *is such that* $\sup(\mathbb{T}) = \infty$*, and the forward operator* $\sigma : \mathbb{T} \to \mathbb{T}$ *is continuous.*

Let G be a finite, edge-weighted graph defined by its finite vertex set VG and the nonnegative weight function $w : VG \times VG \to [t_0, \infty)_{\mathbb{T}}$ with $w \mapsto w_{xy}$ for $x, y \in VG$. We set $w_{xy} = 0$ when there is no edge between x and y. Furthermore, we assume the symmetry that $w_{xy} = w_{yx}$ for all x, y, meaning that the graph is undirected. The graph *Laplace operator* Δ_G is defined for any bounded function $f : VG \to \mathbb{C}$ by

$$\Delta_G f(x) = \sum_{y \in VG} (f(x) - f(y)) w_{xy}. \tag{1.1}$$

Trivially, the Laplace operator is a bounded linear operator on the space of all complex-valued functions defined on VG with the Laplace operator determining the weighted average over the adjacent vertices y, where w_{xy} is the weight value on the edge xy on the graph G. The heat kernel on a weighted graph G in time-scale $\mathbb{T}$ with the base point t_0 is the bounded solution $H_G : V_G \times V_G \times [t_0, \infty)_T \to \mathbb{R}$ to the differential equation

$$\left(\Delta_{G,v_1} + \Delta_t\right) H_G(v_1, v_2; t) = 0, \tag{1.2}$$

subject to the initial condition, which has two possibilities.
If t_0 is right-scattered, meaning $\mu(t_0) > 0$, then

$$H_G(v_1, v_2, t_0) = \begin{cases} 1 & \text{if } v_1 = v_2, \\ 0 & \text{if } v_1 \neq v_2. \end{cases} \tag{1.3}$$

If t_0 is right-dense, meaning $\mu(t_0) = 0$, then

$$\lim_{t \to t_0^+} H_G(v_1, v_2, t) = \begin{cases} 1 & \text{if } v_1 = v_2, \\ 0 & \text{if } v_1 \neq v_2. \end{cases} \tag{1.4}$$

If the graph G is such that the operator $I - \mu(t)\Delta$ is invertible for every $t \in (-\infty, t_0)_{\mathbb{T}}$, then according to [18, Theorem 5.7] or [4, Theorem 8.24] the heat kernel on G exists and is unique (see also discussion on p. 527 of [29]). The proof of the existence and uniqueness of the heat kernel on a graph G when the time-scale $\mathbb{T} = \mathbb{R}$ can be found in [14] and [15]; see also [8] and [7] when the time-scale is $\mathbb{T} = \mathbb{Z}$. Note that if one chooses a basis of functions $f : VG \to \mathbb{C}$, then $I - \mu(t)\Delta$ can be realized by a square matrix $M(t)$ with VG rows and columns. In this instance, the invertibility of $I - \mu(t)\Delta$ is equivalent to the invertibility of $M(t)$.

In this paper, we will prove the existence of $H_G(v_1, v_2, t)$ associated to a fairly general graph G by constructing it explicitly in terms of a certain convolution series; see Theorem 4.7. All graphs G considered in this paper are finite, so that $H_G(v_1, v_2, t)$ can also be expressed as a convergent series associated to the exponential operator $e_{-\Delta_G}(t,t_0)$. We show that for a specific choice of parametrix, namely the Dirac delta, Theorem 4.7 yields the expansion of $e_{-\Delta_G}(t,t_0)$ as a special case; see Example 5.2.

However, in our main theorem, Theorem 4.7, the parametrix used to construct the heat kernel is a fairly general function which allows us to choose, as a starting point in the iterative process of construction, various approximations to the heat kernel under consideration. For example, if our graph G is a subgraph of a graph $\tilde{G}$ for which a closed expression for the heat kernel is known, then one may use the restriction of the heat kernel on $\tilde{G}$ to G as a parametrix. In this case, our main theorem yields an exact formula for the difference $H_G(v_1,v_2,t) - H_{\tilde{G}}(v_1,v_2,t)$.

In particular, when $\tilde{G} = K_N$, the complete graph on N vertices, we obtain the following proposition, which is a closed expression for the heat kernel $H_G(v_1,v_2,t)$ for any subgraph G of K_N.

Proposition 1.1 *Let $N > 1$ be an integer. Assume that $\mathbb{T}$ is any time-scale with a fixed point t_0. Assume that $\sup\mathbb{T} = \infty$ and that $-N$ is regressive in $\mathbb{T}$. Let G be a subgraph of a complete graph K_N on N vertices with all edge weights equal to one. Define the $VG \times VG$ matrix $U_G = (u_G(v_1,v_2))_{|VG|\times|VG|}$ by setting its entries $u_G(v_1,v_2)$ equal to*

$$u_G(v_1,v_2) = \begin{cases} (N-1) - d_G(v_1) & \text{if } v_1 = v_2, \\ -1 & \text{if } v_1 \sim_c v_2, \\ 0 & \text{otherwise,} \end{cases}$$

where $d_G(v_1)$ is the degree of vertex v_1 in G, and the notation $v_1 \sim_c v_2$ denotes that v_1 and v_2 are distinct and disconnected pair of vertices in G. Then the heat kernel H_G on G for all $v_1, v_2 \in VG$ and $t \in [t_0,\infty)_{\mathbb{T}}$ is given by

$$H_G(v_1,v_2;t) = H_{K_N}(v_1,v_2;t) + \sum_{k=1}^{\infty} U_G^k(v_1,v_2) E_{-N,k}(t),$$

where H_{K_N} is the heat kernel on K_N (see equation (5.9) below) and for any $k \geq 1$, we have that

$$E_{-N,k}(t) := \sum_{\ell=0}^{\infty} \binom{\ell+k}{k} (-N)^{\ell} h_{\ell+k}(t,t_0),$$

where $h_k(t,t_0)$ are the basic monomials associated to $\mathbb{T}$, as described in Definition 2.3.

Proposition 1.1 highlights one of the significant features of Theorem 4.7, which we will now discuss a bit further. In general, one can view $\tilde{G}$ as a subgraph of G and use the heat kernel on G as a parametrix for the heat kernel on $\tilde{G}$. In doing so, one obtains an explicit formula for the heat kernel on $\tilde{G}$. One instance is obtained by taking G to be a complete graph, since in that case the heat kernel on a complete graph is explicit. This instance is the contents of Proposition 1.1. In any event, even in the case when the heat kernel on $\tilde{G}$ is not explicitly known, Theorem 4.7 yields a formula for the difference between the heat kernels on G and on $\tilde{G}$; see Example 5.3.

In the setting of Riemannian geometry, there are many studies which investigate comparison theorems for heat kernels, including when one domain is isometrically embedded in another; see for example [10]. We view Example 5.3, as giving the graph and time-scale analogue of the aforementioned comparison theorems since one has an explicit formula for the difference of heat kernels. Also, when the operator $I - \mu(t)\Delta$ is invertible, then by taking different functions as a parametrix, one can use the uniqueness of the heat kernel to deduce identities between different convolution series. An example of such an identity is equation (5.7) from Example 5.4 below.

The organization of this paper is as follows: In Section 2, we introduce the necessary analytic tools for our study. Section 3 establishes the foundational results required for constructing a parametrix. In Section 4, we present the parametrix construction of the heat kernel. Finally, Section 5 gives some applications and illustrative examples of the parametrix and construction of the heat kernel, thus offering insight into the behavior of the heat kernel on finite graphs in various time-scales.

2. Preliminaries

In this section, we recall some results regarding time-scale calculus. Let $\mathbb{T}$ be a time-scale with $\sup(\mathbb{T}) = \infty$, and let $t_0 \in \mathbb{T}$ be a fixed base point. We refer to [4] for definitions of the delta derivative and integral. The notations for delta derivative, $f^{\Delta_t}(t)$ and $\Delta_t f(t)$, are used interchangeably in this paper. We also set $[t_0, t]_{\mathbb{T}} = [t_0, t] \cap \mathbb{T}$, $(t_0, t)_{\mathbb{T}} = (t_0, t) \cap \mathbb{T}$ and similarly for all other variants of subintervals of $\mathbb{T}$.

2.1. Time-scale calculus

For the sake of completeness, we recall from [4] the following two theorems. As stated, for our purposes, we assume that $\sup \mathbb{T} = \infty$, so then $\mathbb{T}^\kappa = \mathbb{T}$. More generally, when $\sup \mathbb{T} < \infty$, we refer to pages 2 of [4] for the definition of $\mathbb{T}^\kappa$, which is a subset of $\mathbb{T}$. Though we are interested in those $\mathbb{T}$ for which $\sup \mathbb{T} = \infty$, we will state the theorems in greater generality.

Theorem 2.1 ([4, Theorem 1.117]) *Let $t_0 \in \mathbb{T}^\kappa$ and assume $f : \mathbb{T} \times \mathbb{T}^\kappa \to \mathbb{R}$ is continuous at (t, t) for $t \in \mathbb{T}^\kappa$ with $t > t_0$. Assume further the following properties.*

(i) The function f is Δ-differentiable as a function of the first variable t, and $f^\Delta(t, .)$ when viewed as a function of the second variable is rd-continuous (right-dense continuous) on $[t_0, \sigma(t)]$.

(ii) For every $\epsilon > 0$, there exists a neighborhood U of t independent of $\tau \in [t_0, \sigma(t)]$ such that

$$|f(\sigma(t), \tau) - f(s, \tau) - f^\Delta(t, \tau)(\sigma(t) - s)| \le \epsilon |\sigma(t) - s|$$

for all $s \in U$.

Then

$$\Delta_t \left(\int_{t_0}^t f(t, \tau) \Delta\tau \right) = \int_{t_0}^t f^\Delta(t, \tau) \Delta\tau + f(\sigma(t), t). \tag{2.1}$$

Theorem 2.2 ([4, Theorem 1.74]) *Every rd-continuous function has an antiderivative. In particular if $t_0 \in \mathbb{T}$, then F defined by*

$$F(t) := \int_{t_0}^t f(\tau) \Delta\tau \quad \textit{for all } t \in \mathbb{T}$$

is an antiderivative of f.

2.2. Class $\mathscr{F}$

We will introduce the basic monomials $h_k(t,s)$ which appear in the Taylor series expansion of delta-differentiable functions and then use those to define a class of functions.

Definition 2.3 *[4] Let $\mathbb{T}$ be any time-scale. The basic monomials are functions $h_k : \mathbb{T}\times\mathbb{T}\to\mathbb{R}$, defined recursively as follows. The first monomial $h_0(t,s)\equiv 1$ for all $s,t\in\mathbb{T}$. For the remaining terms,*

$$h_{k+1}(t,s) := \int_s^t h_k(\tau,s)\Delta\tau.$$

It is proved in [3] that the basic monomials possess the following properties.

(i) For all $t,s\in\mathbb{T}$ and $k\in\mathbb{N}_0$,

$$h_{k+1}^{\Delta_t}(t,s) = h_k(t,s) \text{ and } h_{k+1}^{\Delta_s}(t,s) = -h_k(t,\sigma(s)). \tag{2.2}$$

(ii) For all $k,m\in\mathbb{N}_0$,

$$\int_s^t h_k(t,\sigma(s))h_m(s,t_0)\Delta s = h_{k+m+1}(t,t_0). \tag{2.3}$$

(iii) For all $k\in\mathbb{N}$ and $t,s\in\mathbb{T}$ with $t\geq s$,

$$0\leq h_k(t,s)\leq \frac{(t-s)^k}{k!}. \tag{2.4}$$

Definition 2.4 *[2] Let $\mathbb{T}$ be any time-scale with $\sup(\mathbb{T})=\infty$, and let $t_0\in\mathbb{T}$ be a fixed base point. Let $f:[t_0,\infty)_{\mathbb{T}}\to\mathbb{C}$ be a function. We say f is a function in the class $\mathscr{F}$ if it possesses a series representation of the form*

$$f(t) = \sum_{k=0}^{\infty} a_k h_k(t,t_0) \quad \text{for all } t\in(t_0,\infty]_{\mathbb{T}}, \tag{2.5}$$

where each coefficient a_k in the series is a constant that satisfies the bound

$$|a_k|\leq MR^k \quad \text{for} \quad k\in\mathbb{N}_0 \tag{2.6}$$

for some constants $M>0$ and $R>0$ which are independent of k.

When combining (2.6) with (2.4), it is immediate that the series in (2.5) converges absolutely and uniformly on any compact interval $[t_0,L]_{\mathbb{T}}\subseteq[t_0,\infty)_{\mathbb{T}}$ for any $L\in\mathbb{T}$ with $L\geq t_0$.

Some well-known functions in the class $\mathscr{F}$ are $e_z(t,t_0), \cosh_z(t,t_0), \sinh_z(t,t_0), \cos_z(t,t_0)$ and $\sin_z(t,t_0)$ for any $z\in\mathbb{C}$; see [2]. Another example of functions in the class $\mathscr{F}$ which will be useful in the parametrix construction of the heat kernel in a time-scale $\mathbb{T}$ is the *I-Bessel* function centered at t_0, which is defined as follows.

Example 2.5 *For $n, k \in \mathbb{N}_0$, $c \in \mathbb{C}$ and $t \in \mathbb{T}$, let*

$$I_n^c(t) := \sum_{k=0}^{\infty} \binom{n+2k}{k} \left(\frac{c}{2}\right)^{n+2k} h_{n+2k}(t, t_0). \tag{2.7}$$

We claim that the function $I_n^c(t)$ belongs to the class $\mathscr{F}$. To prove this assertion, it suffices to show that the coefficients in the series expansion satisfies the bound (2.6). Indeed,

$$\left|\binom{n+2k}{k} \left(\frac{c}{2}\right)^{n+2k}\right| \leq \frac{(2|c|)^{n+2k}}{2^{n+2k}} = |c|^{n+2k} \quad \text{for all} \quad k \in \mathbb{N}_0.$$

Therefore, the bound (2.6) holds for all $k \in \mathbb{N}_0$, with $M = |c|^n$ and $R = |c|$.

When $\mathbb{T} = \mathbb{Z}$ and $t_0 = 0$, we see that $I_z(t)$ coincides with the discrete I-Bessel function introduced by Slavík in [28], equation (2.2). Specifically, in this case, $h_{n+2k}(t, t_0) = \binom{t}{n+2k}$, which equals zero unless $k \leq \lfloor (t-n)/2 \rfloor$. Hence,

$$I_n^c(t) = \sum_{k=0}^{\lfloor (t-n)/2 \rfloor} \binom{n+2k}{k} \binom{t}{n+2k} \left(\frac{c}{2}\right)^{n+2k} = \sum_{k=0}^{\lfloor (t-n)/2 \rfloor} \frac{t!}{k!(n+k)!(t-2k-n)!} \left(\frac{c}{2}\right)^{n+2k}. \tag{2.8}$$

According to [8, Proposition 3.2], (2.8) equals the discrete I-Bessel function $I_z^c(t)$; see [28, equation (2.2)] as well as [1] for the case $c = 1$.

We note that the function $I_n^c(t)$ is closely related to the J-Bessel function $J_z(t, s, \xi, \alpha, \gamma; \mathbb{T})$ with $s = t_0$, $\xi = c$, $\gamma = 1$ and $\alpha = 0$ defined on p. 101 of [13].

We now extend the definition of the class $\mathscr{F}$ of functions defined on $[t_0, \infty)_{\mathbb{T}}$ to the class $\mathscr{F}(G)$ of functions defined on $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$ as follows.

Definition 2.6 *Let $\mathbb{T}$ be any time-scale such that the $\sup(\mathbb{T}) = \infty$, and let $t_0 \in \mathbb{T}$ be a fixed base point. Let G be any finite, undirected weighted graph. A function $f : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{C}$ is said to be in the class $\mathscr{F}(G)$ if it possesses a representation of the form*

$$f(v_1, v_2; t) = \sum_{k=0}^{\infty} a_k(v_1, v_2) h_k(t, t_0) \quad \text{for all } t \in (t_0, \infty]_{\mathbb{T}} \quad \text{and} \quad v_1, v_2 \in VG, \tag{2.9}$$

where the coefficient $a_k(v_1, v_2)$ is constant in $\mathbb{T}$ that satisfies the bound

$$|a_k(v_1, v_2)| \leq MR^k \quad \text{for} \quad k \in \mathbb{N}_0 \tag{2.10}$$

for some constants $M > 0$ and $R > 0$ which are independent of k and $v_1, v_2 \in VG$.

2.2.1. Time-scale convolution

In this section, we will recall the definition of the time-scale convolution in [2]. In order to do so, we will first recall the definition of the shift of a function, which is, in full generality, defined as a solution to a certain shifting problem.

Definition 2.7 *[2] For a given $f : [t_0, \infty)_{\mathbb{T}} \to \mathbb{C}$, consider the shifting problem*

$$u^{\Delta_t}(t, \sigma(s)) = -u^{\Delta_s}(t, s), \text{ for any } t \in \mathbb{T}, \text{ with } \ t \geq s \geq t_0,$$

$$u(t, t_0) = f(t), \text{ whenever } t \geq t_0.$$

We let $\hat{f}$ denote a solution to the above differential equation, and we call $\hat{f}$ the shift of f.

Lemma 2.8 ([2, Lemma 2.4, Theorem 5.1.]) *With the notation as above, the following two statements hold true:*

(i) If $\hat{f}$ is the shift of f, then $\hat{f}(t,t) = f(t_0)$ for all $t \in \mathbb{T}$.

(ii) Any function $f \in \mathscr{F}$ has a unique shift in $\mathscr{F}$ which is given by

$$\hat{f}(t, s) = \sum_{k=0}^{\infty} a_k h_k(t, s), \ t \in (t_0, \infty]_{\mathbb{T}}, \ s \in [t_0, t]_{\mathbb{T}}.$$

We now recall the definition of the time-scale convolution of two functions.

Definition 2.9 *[2] Let $f, g : \mathbb{T} \to \mathbb{R}$ be functions such that f possesses the shift $\hat{f}$ and the function $\hat{f}(t, \sigma(s))g(s)$ is delta integrable on any interval $[t_0, t]_{\mathbb{T}}$ for $t \in \mathbb{T}$ with $t \geq t_0$. Then the time-scale convolution is defined as*

$$(f * g)(t) = \int_{t_0}^{t} \hat{f}(t, \sigma(s))g(s)\Delta s.$$

The time-scale convolution is not commutative in general. However, according to [2, Theorem 2.7], it is an associative operation. The distributive property follows immediately from the linearity of the delta integral.

3. Graph convolution

Let $\mathbb{T}$ be any arbitrary time-scale with continuous shift operator. Assume $\sup(\mathbb{T}) = \infty$, and let $t_0 \in \mathbb{T}$ be a fixed base point. Let G be a finite and weighted graph. Let VG be the vertex set of graph G with cardinality $|VG|$. Let $F_1, F_2 : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$ be functions such that the product $\hat{F_1}(v_1, v, t, \sigma(s))F_2(v, v_2; s)$ when viewed as function of variable $s \in \mathbb{T}$ is integrable on every interval $[t_0, t]_{\mathbb{T}} \subseteq \mathbb{T}$ with $t \geq s \geq t_0$ and any $v_1, v_2, v \in VG$.

Definition 3.1 *The graph convolution of functions F_1 and F_2 is defined as*

$$(F_1 *_G F_2)(v_1, v_2; t) := \int_{t_0}^{t} \sum_{v \in VG} \hat{F_1}(v_1, v; t, \sigma(s))F_2(v, v_2; s)\Delta s. \tag{3.1}$$

One can view F_1 and F_2 as operators on $L^2(VG)$. If one chooses a basis of $L^2(VG)$, then F_1 and F_2 can be represented as matrices, in which case, one can write

$$(F_1 *_G F_2)(t) := \int_{t_0}^{t} \hat{F}_1(t,\sigma(s)) \cdot F_2(s)\Delta s,$$

where $\cdot$ signifies matrix multiplication. Also, we can view graph convolution as a sum of time convolutions over the vertex set VG. In general, graph convolution is not a commutative operation, but it does inherit the associative and distributive properties from time-scale convolution. Specifically, for $F_i(v_1,v_2;t), i=1,2,3, F_i : VG \times VG \times \mathbb{T} \to \mathbb{R}$, we have the following identities:

$$[(F_1 *_G F_2) *_G F_3](v_1,v_2;t) = [F_1 *_G (F_2 *_G F_3)](v_1,v_2;t),$$

$$[F_1 *_G (F_2 + F_3)](v_1,v_2;t) = (F_1 *_G F_2)(v_1,v_2;t) + (F_1 *_G F_3)(v_1,v_2;t),$$
$$[(F_1 + F_2) *_G F_3)](v_1,v_2;t) = (F_1 *_G F_3)(v_1,v_2;t) + (F_2 *_G F_3)(v_1,v_2;t).$$

For these formulas, we assume that each function in question has a shift, and the necessary conditions on integrability are true.

Going further, we have the following lemmas.

Lemma 3.2 *Let $F_1, F_2 : VG \times VG \times [t_0,\infty)_{\mathbb{T}} \to \mathbb{R}$ be as above. Assume further there exist constants $C_1, C_2 \geq 0$ and integers $k, m \geq 0$ such that for all $t, s \in [t_0,\infty)_{\mathbb{T}}$ with $t \geq s \geq t_0$ and $v_1, v_2 \in VG$, we have the bounds that*

$$|\hat{F}_1(v_1,v;t,s)| \leq C_1 h_k(t,s) \quad \text{and} \quad |F_2(v,v_2;t)| \leq C_2 h_m(t,t_0).$$

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

$$|(F_1 *_G F_2)(v_1,v_2;t)| \leq C_1 C_2 |VG| h_{k+m+1}(t,t_0).$$

Proof The proof follows from the definition of graph convolution and an application of the basic monomial formula (2.3). □

Lemma 3.3 *Assume $f : VG \times VG \times [t_0,\infty)_{\mathbb{T}} \to \mathbb{R}$ is such that $\hat{f}$ exists. For each integer $\ell > 0$, assume that the ℓ-fold graph convolution of f exists on the interval $[t_0,t]_{\mathbb{T}}$. Furthermore, consider three possible additional assumptions on f.*

(i) There exist some constants $C, \hat{C} \geq 0$ such that

$$|f(v_1,v_2;t)| \leq C \text{ and } |\hat{f}(v_1,v_2;t,s)| \leq \hat{C}$$

for all $v_1, v_2 \in VG, t, s \in \mathbb{T}$, with $t \geq s \geq t_0$.

(ii) There exist some constants $C_1, C_2, \hat{C}_1, \hat{C}_2$, and integers $k, m \geq 0$ such that

$$|f(v_1,v_2;t)| \leq C_1 + C_2 h_k(t,t_0) \text{ and } |\hat{f}(v_1,v_2;t,s)| \leq \hat{C}_1 + \hat{C}_2 h_m(t,s)$$

for all $v_1, v_2 \in VG, t, s \in \mathbb{T}$, with $t \geq s \geq t_0$.

(iii) For all $v_1, v_2 \in VG$*, the functions* $f(v_1, v_2; t)$ *and* $\hat{f}(v_1, v_2; t, s)$ *are continuous for any* $t, s \in [t_0, \infty)_{\mathbb{T}}$ *with* $t \geq s \geq t_0$*.*

If any of the assumptions (i), (ii) or (iii) hold, then the series

$$\sum_{\ell=1}^{\infty} (-1)^{\ell} (f)^{*_G \ell}(v_1, v_2; t) \tag{3.2}$$

converges absolutely and uniformly on every compact subset of $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$*. In addition, we have that*

$$\left(f *_G \sum_{\ell=1}^{\infty} (-1)^{\ell} (f)^{*_G \ell} \right)(v_1, v_2; t) = \sum_{\ell=1}^{\infty} (-1)^{\ell} (f)^{*_G (\ell+1)}(v_1, v_2; t). \tag{3.3}$$

Proof Let us begin with assumption (i). With the given assumptions, we apply Lemma 3.2 to get that

$$(f *_G f)(v_1, v_2; t) \leq C\hat{C}|VG| h_0(t, t_0).$$

Then by induction on $\ell \geq 1$, by applying properties (2.3) and (2.4) of the basic monomials, we obtain that

$$\left| (f)^{*_G \ell}(v_1, v_2, t) \right| \leq C\hat{C}^{\ell-1} |VG|^{\ell-1} \frac{(T - t_0)^{\ell-1}}{(\ell-1)!}.$$

With the given bound, our series converges by the Weierstrass criterion. For a fixed $t > 0$, by the approach above, the series on the right-hand side converges absolutely. Then, by integrating term-wise, we have

$$\left(f *_G \sum_{\ell=1}^{\infty} (-1)^{\ell} (f)^{*_G \ell} \right)(v_1, v_2; t) = \sum_{\ell=1}^{\infty} (-1)^{\ell} \int_{t_0}^{t} \sum_{v \in VG} \left(\hat{f}(v_1, v; t, \sigma(s)) (f)^{*_G \ell}(v, v_2; s) \right) \Delta s,$$

thus establishing (3.3).

Under the assumption of (ii), for a fixed compact subset $A \subseteq VG \times VG \times [t_0, \infty)_{\mathbb{T}}$, assumption (ii) combined with inequality (2.4) yields that

$$|f(v_1, v_2; t)| \leq \tilde{C}(T - t_0)^k \quad \text{and} \quad |f(v_1, \hat{v_2}; t, s)| \leq \hat{\tilde{C}}(T - t_0)^m,$$

for some constants $\tilde{C}, \hat{\tilde{C}} \geq 0$, and for all $(v_1, v_2, t) \in A$ with $t \geq s \geq t_0$. For assumption (iii), the boundedness of $f(v_1, v_2, t)$ and $\hat{f}(v_1, v_2; t, s)$ then follows from continuity. In both cases, the proof of the assertion follows by arguing as in the proof under condition (i).

□

Remark 3.4 *Every function* $f \in \mathscr{F}(G)$ *is continuous when viewed as a function of* $t \in [t_0, \infty)_{\mathbb{T}}$*, as an absolutely and uniformly convergent series of continuous functions. Moreover, for* $f \in \mathscr{F}(G)$ *such that*

$$f(v_1, v_2; t) = \sum_{k=0}^{\infty} a_k(v_1, v_2) h_k(t, t_0),$$

we have

$$\hat{f}(v_1, v_2; t, s) = \sum_{k=0}^{\infty} a_k(v_1, v_2) h_k(t, s),$$

which is also a continuous function for all $v_1, v_2 \in VG, t, s \in (t_0, \infty]$ *with* $t \geq s \geq t_0$*. Therefore, Lemma 3.3 holds true for every* $f \in \mathscr{F}(G)$*.*

4. The parametrix construction of the heat kernel

In this section, we will give a series representation of the heat kernel of an undirected, weighted and finite graph G in Time-scale $\mathbb{T}$ with $\sup(\mathbb{T}) = \infty$ and $t_0 \in \mathbb{T}$ is a fixed base point. We start by introducing the heat operator.

Definition 4.1 *Let* $f : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{C}$ *be a differentiable function in variable* t *for any choice of the space variables from* VG*. The heat operator* L_{v_1} *is a linear operator defined on the space* $L^2(VG \times VG \times [t_0, \infty)_{\mathbb{T}})$ *of complex-valued functions by its action on function* $f(v_1, v_2; t)$ *in the first variable* v_1*, given by*

$$(L_{v_1} f)(v_1, v_2; t) := ((\Delta_{G,v_1} + \Delta_t) f)(v_1, v_2; t). \tag{4.1}$$

We now define a parametrix for the heat kernel, which is a function satisfying reasonably general conditions, as now specified.

Definition 4.2 *A* parametrix *for the heat operator on a graph* G *in time-scale* $\mathbb{T}$ *is any function* $f : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$*, which satisifes the following conditions.*

1. *For all* $v_1, v_2 \in VG$*, the function* $f(v_1, v_2, t)$ *is continuous in variable* t *on* $[t_0, \infty)_{\mathbb{T}}$ *and continuously differentiable in variable* t *on* $(t_0, \infty)_{\mathbb{T}}$ *such that* $f^{\Delta_t}(v_1, v_2, t)$ *extends to a continuous function on* $[t_0, \infty)_{\mathbb{T}}$.

2. *Let* $v_1, v_2 \in VG$*.*

   (i) The function $\hat{f}(v_1, v_2, t, s)$ *is continuous at any ordered pair* (t, s) *for* $t \geq s \geq t_0$*;* $\hat{f}(v_1, v_2, t, s)$ *is continuously differentiable in variables* t *and* s *for* $t > s > t_0$*. Moreover,* $\hat{f}^{\Delta_t}(v_1, v_2, t, s)$ *extends to a continuous function on* $[t_0, \infty)_{\mathbb{T}}$*, and* $\hat{f}^{\Delta_s}(v_1, v_2, t, s)$ *extends to a continuous function on* $[t_0, t]_{\mathbb{T}}$.

   (ii) The functions $\hat{f}^{\Delta_t}(v_1, v_2, t, s)$ *and* $\hat{f}^{\Delta_s}(v_1, v_2, t, s)$ *are* Δ_s *and* Δ_t *differentiable respectively, for* $t > s > t_0$*. The mixed second partial derivatives* $\hat{f}^{\Delta_t \Delta_s}(v_1, v_2, t, s)$ *and* $\hat{f}^{\Delta_s \Delta_t}(v_1, v_2, t, s)$ *possess continuous extensions to the boundary points of the intervals of definition, and* $\hat{f}^{\Delta_t \Delta_s}(v_1, v_2, t, s) = \hat{f}^{\Delta_s \Delta_t}(v_1, v_2, t, s)$ *for all* $t \geq s \geq t_0$*.*

3. *(Dirac delta condition) If* t_0 *is right-scattered, then*

$$f(v_1, v_2, t_0) = \begin{cases} 1 & \text{if } v_1 = v_2, \\ 0 & \text{if } v_1 \neq v_2, \end{cases} \tag{4.2}$$

whereas if t_0 is right-dense then

$$\lim_{t\to t_0{}^+} f(v_1, v_2, t) = \begin{cases} 1 & \text{if } v_1 = v_2, \\ 0 & \text{if } v_1 \neq v_2. \end{cases} \tag{4.3}$$

Example 4.3 *The properties of a parametrix, when viewed as a function of the time variable $t \in \mathbb{T}$, are stated in the first two conditions of Definition 4.2 and are fulfilled by any function $f \in \mathscr{F}(G)$. As a result, we may consider those conditions to be reasonably general. Namely, for any $v_1, v_2 \in VG$, the function $f(v_1, v_2; t) \in \mathscr{F}$ is defined as an absolutely and uniformly convergent series involving the basic monomials, so then according to Lemma 2.8 so is $\hat{f}(v_1, v_2; t, s)$. By applying properties (2.2) and (2.3) of the basic monomials, it is straightforward to conclude that conditions 1 and 2 of Definition 4.2 are satisfied.*

Proposition 4.4 *Let $f : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$ be a parametrix for the heat operator on a graph G in time-scale $\mathbb{T}$. Let $g : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$ be any continuous function on $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$. Then*

$$(f *_G g)^{\Delta_t}(v_1, v_2; t) = (f^{\Delta_t} *_G g)(v_1, v_2; t) + g(v_1, v_2; t).$$

Proof

The assumptions on the parametrix f, together with the continuity of the shift operator yield that assumptions of Theorem 2.1 are all met. By applying Theorem 2.1 (ii) and Lemma 2.8 (i), we deduce that

$$\begin{aligned}
(f *_G g)^{\Delta_t}(v_1, v_2; t) &= \sum_{v\in VG} \Delta_t \left(\int_{t_0}^{t} \hat{f}(v_1, v; t, \sigma(s)) g(v, v_2; s) \Delta s \right) \\
&= \sum_{v\in VG} \left[\int_{t_0}^{t} \Delta_t \left(\hat{f}(v_1, v; t, \sigma(s)) g(v, v_2; s) \right) \Delta s + \hat{f}(v_1, v; \sigma(t), \sigma(t)) g(v, v_2; t) \right] \\
&= \sum_{v\in VG} \left[\int_{t_0}^{t} \Delta_t \left(\hat{f}(v_1, v; t, \sigma(s)) g(v, v_2; s) \right) \Delta s + f(v_1, v; t_0) g(v, v_2; t) \right].
\end{aligned}$$

Condition (ii) of the parametrix f ensures the equality of mixed partial delta derivatives of $\hat{f}$ in s and t, which, in turn yields that $\hat{f}^{\Delta_t} = \widehat{f^{\Delta_t}}$. Therefore,

$$(f *_G g)^{\Delta_t}(v_1, v_2; t) = \sum_{v\in VG} \left[\int_{t_0}^{t} \widehat{f^{\Delta_t}}(v_1, v; t, \sigma(s)) g(v, v_2; s) \Delta s + f(v_1, v; t_0) g(v, v_2; t) \right].$$

From the Dirac delta condition fulfilled by the parametrix f, we have that

$$\begin{aligned}
(f *_G g)^{\Delta_t}(v_1, v_2; t) &= \sum_{v\in VG} \left[\int_{t_0}^{t} \widehat{f^{\Delta_t}}(v_1, v; t, \sigma(s)) g(v, v_2; s) \Delta s \right] + g(v_1, v_2; t) \\
&= (f^{\Delta_t} *_G g) + g(v_1, v_2; t),
\end{aligned}$$

which completes the proof. □

Proposition 4.5 *Let $f : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$ be a parametrix for the heat operator on a graph G in time-scale $\mathbb{T}$. Let $g : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$ be any continuous function on $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$. Then*

$$\Delta_{G,v_1}(f *_G g)(v_1, v_2; t) = (\Delta_{G,v_1} f *_G g)(v_1, v_2; t).$$

Proof By the definition of the Laplace operator and graph convolution, we have that

$$\begin{aligned}\Delta_{G,v_1}(f *_G g)(v_1, v_2; t) &= \sum_{y\in VG} ((f *_G g)(v_1, v_2; t) - (f *_G g)(y, v_2; t))\, w_{v_1 y} \\ &= \sum_{v\in VG} \int_{t_0}^{t} \sum_{y\in VG} \Big(\hat{f}(v_1, v; t, \sigma(s) - \hat{f}(y, v; t, \sigma(s)\Big)\, w_{v_1 y} g(v, v_2; s)\Delta s \\ &= \sum_{v\in VG} \int_{t_0}^{t} \Delta_{G,v_1} \hat{f}(v_1, v; t, \sigma(s)) g(v, v_2; s)\Delta s.\end{aligned}$$

Note that the shift of a linear combination of functions is equal to the linear combination of shifts. Hence,

$$\begin{aligned}\Delta_{G,v_1}(f *_G g)(v_1, v_2; t) &= \sum_{v\in VG} \int_{t_0}^{t} \widehat{\Delta_{G,v_1}} f(v_1, v; t, \sigma(s)) g(v, v_2; s)\Delta s \\ &= (\Delta_{G,v_1} f *_G g)(v_1, v_2; t).\end{aligned}$$

□

Lemma 4.6 *Let* $f : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$ *be a parametrix for the heat operator on a graph* G *in time-scale* $\mathbb{T}$*. Let* $g : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$ *be any continuous function on* $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$*. Then*

$$L_{v_1}(f *_G g)(v_1, v_2; t) = (L_{v_1} f *_G g)(v_1, v_2; t) + g(v_1, v_2; t).$$

Proof The proof follows from the definition of the operator L_{v_1} together with Propositions 4.4 and 4.5. □

Theorem 4.7 *Let* $f : VG \times VG \times [t_0, \infty)_{\mathbb{T}} \to \mathbb{R}$ *be a parametrix for the heat operator on a graph* G *in time-scale* $\mathbb{T}$*. For all* $v_1, v_2 \in VG$ *and* $t \in [t_0, \infty)_{\mathbb{T}}$*, define*

$$F(v_1, v_2; t) := \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} f)^{*_G \ell}(v_1, v_2; t). \tag{4.4}$$

Then F *is a continuous function on* $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$ *and*

$$H_G(v_1, v_2; t) = f(v_1, v_2; t) + (f *_G F)(v_1, v_2; t) \tag{4.5}$$

is the heat kernel on G *in time-scale* $\mathbb{T}$*.*

Proof Recall that assumptions 1. and 2. from Definition 4.2 imply that $(\hat{f})^{\Delta_t} = \widehat{f^{\Delta_t}}$ and $\widehat{\Delta_{G,v_1}} f = \Delta_{G,v_1} \hat{f}$, and these functions are continuous. Therefore, the function $\widehat{L_{v_1} f}$ is continuous, which, when combined with the continuity of $L_{v_1} f$ and Theorem 2.2 yield that the 2−fold graph convolution $(L_{v_1} f *_G L_{v_1} f)(v_1, v_2; t)$ is a differentiable function of time variable t, hence continuous. By induction on ℓ, the same holds true for $(L_{v_1} f)^{*_G \ell}$. Lemma 3.3 part (iii) ensures uniform convergence of the series on the right-hand side of (4.4) on any compact subsets of $VG \times VG \times [t_0, \infty)\mathbb{T}$, hence the function F as defined in 4.4 is a continuous function.

We will now show the function $H_G(v_1, v_2; t)$ satisfies the Dirac delta condition. When t_0 is right-scattered, then $(f *_G F)(v_1, v_2; t_0) = 0$, so then

$$H_G(v_1, v_2; t_0) = f(v_1, v_2; t_0) + (f *_G F)(v_1, v_2; t_0) = f(v_1, v_2; t_0).$$

When t_0 is right-dense, the continuity of $\hat{f}$ and F implies that $\lim_{t\to t_0{}^+}(f *_G F)(v_1, v_2; t) = 0$. Hence, when passing to the limit $t \to t_0{}^+$ in the definition (4.5) of H_G, we deduce that

$$\lim_{t\to t_0{}^+} H_G(v_1, v_2, t) = \lim_{t\to t_0{}^+} f(v_1, v_2, t).$$

It remains to show $L_{v_1} H_G(v_1, v_2; t) = 0$ for all $v_1, v_2 \in VG$ and $t \in [t_0, \infty)_{\mathbb{T}}$. By Lemma 4.6, we have that

$$\begin{aligned} L_{v_1} H_G(v_1, v_2; t) &= L_{v_1} f(v_1, v_2; t) + L_{v_1}(f *_G F)(v_1, v_2, t) \\ &= L_{v_1} f(v_1, v_2; t) + (L_{v_1} f *_G F)(v_1, v_2; t) + F(v_1, v_2; t). \end{aligned}$$

By applying equation (3.3) of Lemma 3.3 and using the absolute convergence of the two series, we deduce that

$$\begin{aligned} L_{v_1} H_G(v_1, v_2; t) = L_{v_1} f(v_1, v_2; t) &+ \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} f)^{*_G \ell+1}(v_1, v_2; t) \\ &+ \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} f)^{*_G \ell}(v_1, v_2; t) = 0. \end{aligned}$$

With all this, the proof of the theorem is complete. □

5. Applications

Let us now illustrate the applicability of our results. We will present a few examples of a parametrix and show how to deduce heat kernels associated to these choices. First, we discuss applications for general graphs and then we specialize our results to the setting of a complete graph on N vertices.

5.1. Choosing a parametrix from $\mathscr{F}(G)$

The following general result shows that if one can construct the heat kernel on G by starting with a parametrix from $\mathscr{F}(G)$, then the heat kernel will also belong to $\mathscr{F}(G)$.

Proposition 5.1 *With the notation as above, let f be a parametrix for the heat kernel H_G on a finite, undirected, weighted graph G in time-scale $\mathbb{T}$, with the fixed base point t_0. If $f \in \mathscr{F}(G)$, then $H_G \in \mathscr{F}(G)$.*

Proof From [2, Theorem 5.3], we have that for any two functions in $\mathscr{F}(G)$, their convolution belongs to $\mathscr{F}(G)$. Hence, in order to prove the proposition, it suffices to show that the function F defined by (4.4) belongs to $\mathscr{F}(G)$. Let

$$f(v_1, v_2; t) = \sum_{k=0}^{\infty} a_k(v_1, v_2) h_k(t, t_0)$$

with $|a_k(v_1, v_2)| \leq MR^k$, for some constants M, R and all $v_1, v_2 \in VG$, $k \in \mathbb{N}_0$. Since $\Delta_t h_k(t, t_0) = h_{k-1}(t, t_0)$ for $k \geq 1$, we have that

$$g(v_1, v_2; t) := L_{v_1} f(v_1, v_2; t) = \sum_{k=0}^{\infty} \left(\sum_{v\sim v_1} (a_k(v_1, v_2) - a_k(v, v_2)) w_{v_1 v} + a_{k+1}(v_1, v_2) \right) h_k(t, t_0).$$

Therefore,

$$g(v_1, v_2; t) = \sum_{k=0}^{\infty} b_k(v_1, v_2) h_k(t, t_0)$$

with

$$|b_k(v_1, v_2)| \le C(G) R^{k+1} \quad \text{for all} \quad v_1, v_2 \in VG \quad \text{and} \quad k \in \mathbb{N}_0. \tag{5.1}$$

The constant $C(G)$ in 5.1 depends solely on f and G. By combining [2, Theorem 5.3] with the definition of the graph convolution, we get that

$$(g *_G g)(v_1, v_2; t) = \sum_{k=1}^{\infty} b_k^{(1)}(v_1, v_2) h_k(t, t_0),$$

where

$$b_k^{(1)}(v_1, v_2) = \sum_{v \in VG} \sum_{j=0}^{k-1} b_j(v_1, v) b_{k-1-j}(v, v_2).$$

From (5.1), it follows that

$$|b_k^{(1)}(v_1, v_2)| \le |VG| C(G)^2 k R^{k+1}, \text{ for all } v_1, v_2 \in VG \text{ and } k \in \mathbb{N}_0. \tag{5.2}$$

By applying [2, Theorem 5.3] combined with (5.1), (5.2) and the definition of the graph convolution, we deduce that

$$g *_G (g *_G g)(v_1, v_2; t) = \sum_{k=2}^{\infty} b_k^{(2)}(v_1, v_2) h_k(t, t_0),$$

where

$$|b_k^{(2)}(v_1, v_2)| \le |VG|^2 C(G)^3 \binom{k}{2} R^{k+1}, \text{ for all } v_1, v_2 \in VG, \ k \in \mathbb{N}_0.$$

Proceeding by induction on ℓ, one now easily deduces that

$$(g)^{*_G \ell}(v_1, v_2; t) = \sum_{k=\ell}^{\infty} b_k^{(\ell)}(v_1, v_2) h_k(t, t_0)$$

where

$$|b_k^{(\ell)}(v_1, v_2)| \le |VG|^{\ell} C(G)^{\ell+1} \binom{k}{\ell} R^{k+1}, \text{ for all } v_1, v_2 \in VG \text{ and } k \in \mathbb{N}_0. \tag{5.3}$$

Notice that for fixed $n \in \mathbb{N}$ the basic monomial h_n appears in the series expansion of $(g)^{*_G \ell}(v_1, v_2; t)$ only for $\ell \le n$. Therefore, we can write that

$$F(v_1, v_2; t) = \sum_{\ell=1}^{\infty} (-1)^{\ell} (g)^{*_G \ell}(v_1, v_2; t) = \sum_{k=1}^{\infty} A_k(v_1, v_2) h_k(t, t_0),$$

where

$$A_k(v_1, v_2) = \sum_{\ell=1}^{k} (-1)^{\ell} b_k^{(\ell)}(v_1, v_2).$$

From (5.3), we have that

$$|A_k(v_1,v_2)| \le \sum_{\ell=1}^{k} |VG|^{\ell} C(G)^{\ell+1} \binom{k}{\ell} R^{k+1} \le C(G)R[R(1+|VG|C(G))]^k$$

for all $v_1, v_2 \in VG$ and $k \in \mathbb{N}_0$. This proves that F defined by (4.4) belongs to $\mathscr{F}(G)$ and completes the proof of the proposition. □

5.2. Dirac delta as a parametrix

In a sense, the simplest parametrix is the Dirac delta function. As it turns out, the parametrix construction of the heat kernel starting with the Dirac delta function as a parametrix yields the classical expression $e_{-\Delta_G}(t,t_0)$ for the heat kernel.

Example 5.2 *The Dirac delta function is defined as*

$$f(v_1,v_2;t) := \delta_{v_1=v_2} = \begin{cases} 1 & \text{if } v_1 = v_2, \\ 0 & \text{if } v_1 \ne v_2, \end{cases} \quad \text{for all } t \in [t_0,\infty)_{\mathbb{T}}. \tag{5.4}$$

Obviously, $f(v_1,v_2;t)$ satisfies all three conditions in the definition of the parametrix. Furthermore, the shift of $f(v_1,v_2;t)$ is precisely $\delta_{v_1=v_2}$. Therefore,

$$\begin{aligned} L_{v_1} f(v_1,v_2;t) &= \sum_{v\sim v_1} (f(v_1,v_2;t) - f(v,v_2;t)) w_{v_1,v} + \Delta_t f(v_1,v_2;t) \\ &= \sum_{v\sim v_1} (\delta_{v_1=v_2} - \delta_{v=v_2}) w_{v_1,v} \\ &= \begin{cases} d(v_1) & \text{if } v_1 = v_2, \\ -w_{v_1,v_2} & \text{if } v_1 \sim v_2, \\ 0 & \text{otherwise,} \end{cases} \end{aligned}$$

where $d(v_1) = \sum_{v\sim v_1} w_{vv_1}$ is the degree of the vertex v_1. Clearly, $L_{v_1} f(v_1,v_2;t)$ is a constant function in t. By induction on ℓ, we get that

$$(f *_G (L_{v_1} f)^{*_G \ell+1})(v_1,v_2;t) = \Delta_G^{\ell}(v_1,v_2) h_\ell(t,t_0),$$

where $\Delta_G^{\ell}(v_1,v_2)$ is the v_1,v_2 entry of ℓ^{th} exponentiation of graph Lapacian. By envoking Theorem 4.7 we get that

$$\begin{aligned} H_G(v_1,v_2;t) &= f(v_1,v_2;t) + \sum_{\ell=1}^{\infty} (-1)^{\ell} (f *_G (L_{v_1} f)^{*_G \ell})(v_1,v_2;t) \\ &= \delta_{v_1=v_2} + \sum_{\ell=1}^{\infty} (-1)^{\ell} \sum_{v\in VG} \int_{t_0}^{t} \delta_{v_1=v} \cdot \Delta_G^{\ell}(v,v_2) h_\ell(t,t_0) \Delta s \\ &= \delta_{v_1=v_2} + \sum_{\ell=1}^{\infty} (-1)^{\ell} \Delta_G^{\ell}(v_1,v_2) h_\ell(t,t_0). \end{aligned}$$

By definition, set Δ_G^0 *to be the identity matrix. Then, we can write the heat kernel as*

$$H_G(v_1, v_2; t) = \sum_{\ell=0}^{\infty} (-1)^\ell \Delta_G^\ell(v_1, v_2) h_\ell(t, t_0) = e_{-\Delta_G}(t, t_0); \tag{5.5}$$

see [29], equation (2.3) with $A = -\Delta_G$.

It is immediate from (5.5) that the heat kernel H_G *is an element of* $\mathscr{F}(G)$.

5.3. Comparing heat kernels on a graph and from a subgraph

In a sense, the result in the above example was obtained by using the most elementary choice for a parametrix. Of course, there are many other possible choices depending on the setup, which may provide a better approximation to the heat kernel, at least in time variable, than the Dirac delta. In the computations below, we consider the setting when one has the structure of a graph G which is a subgraph of $\tilde{G}$, and we obtain a precise formula for the difference of heat kernels $H_G - H_{\tilde{G}}$.

Example 5.3 *As stated, assume that the graph* G *is a subgraph of some graph* $\tilde{G}$. *If the heat kernel* $H_{\tilde{G}}$ *on* $\tilde{G}$ *is, in a sense, known, then its restriction to* G *may serve as a parametrix for construction of the heat kernel on* G. *Proposition 5.1 implies that* $H_{\tilde{G}}$, *when viewed as a function on* $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$ *belongs to the class* $\mathscr{F}(G)$, *hence satisfies the first two conditions in the definition of the parametrix. The third condition is fulfilled because* $H_{\tilde{G}}$ *is the heat kernel on* $\tilde{G}$. *Referring to Theorem 4.7, let us take* f *to be the restriction of* $H_{\tilde{G}}$ *to* $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$. *When doing so, we obtain the following formula*

$$H_G(v_1, v_2; t) - H_{\tilde{G}}(v_1, v_2; t) = (H_{\tilde{G}} *_G F)(v_1, v_2; t), \tag{5.6}$$

where

$$F(v_1, v_2; t) = \sum_{\ell=1}^{\infty} (-1)^\ell (L_{v_1} H_{\tilde{G}})^{*_G \ell}(v_1, v_2; t).$$

Observe that (5.6) is a precise relation for the difference of the heat kernels H_G *and* $H_{\tilde{G}}$, *when restricted to* G.

The flexibility to choose a rather general function as a parametrix allows us to deduce many identities, which stem from the uniqueness property of the heat kernel under an additional assumption that the operator $I - \mu(t)\Delta_G$ is invertible. Specifically, by starting with two different choices of parametrix, we obtain two different expressions for the heat kernel, and these two expressions must be equal to each other due to uniqueness of the heat kernel. In the case of the real time-scale, such considerations yield a proof of the classical theta inversion formula and Poisson summation; see [22]. It remains to be seen what additional identities arise from considering other time-scales.

In the example below, we discuss a choice for the parametrix different from the Dirac delta, in the case when G is finite, weighted, and connected graph.

Example 5.4 *Assume that* G *is finite, weighted, and connected graph with no loops, meaning that* $w_{vv} = 0$ *for all* $v \in VG$. *Let* d_G *denotes the combinatorial graph distance which is defined as follows. For any two vertices* $v_1, v_2 \in VG$, *set* $d_G(v_1, v_2)$ *be the minimal number of edges in a path connecting* v_1 *and* v_2. *Such a path must* *exist because G is connected. Let I_n^c denote the I-Bessel function in time-scale defined by (2.7). Then for any $c \in \mathbb{C}$, the function*

$$f(v_1, v_2; t) := I^c_{d_G(v_1,v_2)}(t), \quad v_1, v_2 \in VG, t \in [t_0, \infty)_{\mathbb{T}},$$

is a parametrix for the heat kernel on G. This function belongs to the class $\mathscr{F}(G)$, hence fulfills the first two conditions for the parametrix. Moreover, for $t = t_0$ in the case when t_0 is right-scattered we have $h_j(t, t_0) = 0$ unless $j = 0$ in which case $h_j(t_0, t_0) = h_0(t_0, t_0) = 1$. Analogously, in the case when t_0 is right-dense, we have $\lim_{t\to t_0^+} h_j(t, t_0) = 0$ unless $j = 0$, in which case $\lim_{t\to t_0^+} h_0(t, t_0) = 1$. Therefore, $f(v_1, v_2; t_0) = 0$ unless $d_G(v_1, v_2) = 0$, in which case one must have $v_1 = v_2$ and $f(v_1, v_2; t_0) = f(v_1, v_1; t_0) = 1$.

Assume further that the operator $I - \mu(t)\Delta_G$ is invertible. Then we may use the uniqueness of the heat kernel to deduce that

$$\sum_{\ell=0}^{\infty}(-1)^\ell \Delta_G^\ell(v_1, v_2)h_\ell(t, t_0) = f(v_1, v_2; t) + \sum_{\ell=1}^{\infty}(-1)^\ell (f *_G (L_{v_1} f)^{*_G \ell})(v_1, v_2; t), \tag{5.7}$$

which is valid for all $v_1, v_2 \in VG$, $t \in [t_0, \infty)_{\mathbb{T}}$. Equation (5.7) gives an interesting relation between time-scale I-Bessel function (2.7) and the basic monomials from Definition 2.3.

5.4. Specialization to the complete graph on N vertices

Let us further specialize our results by taking $G = K_N$, the complete graph with N vertices and $N(N-1)/2$ edges, with each edge having the weight equal to one. We will give an illustration of the parametrix construction by taking the heat kernel on K_N as a parametrix to compute the heat kernel on its subgraph G. The additional restriction posed on $\mathbb{T}$ is the assumption that the constant $-N$ is regressive in $\mathbb{T}$, meaning that $1 - N\mu(t) \neq 0$ for all $t \in \mathbb{T}^\kappa$.

For any integer $\ell > 0$, the entries for the ℓ-th power of the graph Laplacian on K_N are

$$\Delta^\ell(v_1, v_2) = \begin{cases} N^{\ell-1}(N-1) & \text{if } v_1 = v_2, \\ -N^{\ell-1} & \text{if } v_1 \neq v_2. \end{cases} \tag{5.8}$$

Let us employ the notation of exponential function from [2]. By (5.8) and (5.5), a straightforward computation obtains an explicit expression for the heat kernel on K_N in time-scale $\mathbb{T}$, namely that

$$H_{K_N}(v_1, v_2; t) = \begin{cases} \frac{1}{N} + (1 - \frac{1}{N})e_{-N}(t, t_0) & \text{if } v_1 = v_2, \\ \frac{1}{N} - \frac{1}{N}e_{-N}(t, t_0) & \text{if } v_1 \neq v_2. \end{cases} \tag{5.9}$$

We find it interesting to see the evaluations of (5.9) in different time-scales. Reference [4] gave several examples of exponential functions for various time-scales which can now be used.

When $\mathbb{T} = \mathbb{R}$ and base point $t_0 = 0$, we have that

$$H_{K_N}(v_1, v_2; t) = \begin{cases} \frac{1}{N} + (1 - \frac{1}{N})e^{-Nt} & \text{if } v_1 = v_2, \\ \frac{1}{N} - \frac{1}{N}e^{-Nt} & \text{if } v_1 \neq v_2, \end{cases}$$

which coincides with the formula from [23].

When $\mathbb{T} = h\mathbb{Z}$ for $h > 0$ and $t_0 = 0,$, we get that

$$H_{K_N}(v_1, v_2; t) = \begin{cases} \frac{1}{N} + (1 - \frac{1}{N})(1 - Nh)^{t/h} & \text{if } v_1 = v_2, \\ \frac{1}{N} - \frac{1}{N}(1 - Nh)^{t/h} & \text{if } v_1 \neq v_2. \end{cases}$$

Thus, we have an explicit formula for the heat kernel of K_N in the time-scale $h\mathbb{Z}$.

Let H_n be the so-called harmonic numbers, namely

$$H_0 = 0 \text{ and } H_n = \sum_{k=1}^{n} \frac{1}{k} \text{ for } n \in \mathbb{N}.$$

Consider the time-scale $\mathbb{T} = \{H_n : n \in \mathbb{N}_0\}$ and set $t_0 = 0$. Then the exponential function $e_{-N}(H_n, 0) = \binom{n-N}{n}$. Hence, the heat kernel of K_N is given by

$$H_{K_N}(v_1 v_2; t) = \begin{cases} \frac{1}{N} + (1 - \frac{1}{N})\binom{n-N}{n} & \text{if } v_1 = v_2, \\ \frac{1}{N} - \frac{1}{N}\binom{n-N}{n} & \text{if } v_1 \neq v_2. \end{cases}$$

Let $\mathbb{T} = q^{\mathbb{N}_0}$ with $q > 1$ be the quantum time-scale. Let $t_0 = 1$. Then

$$H_{K_N}(v_1, v_2; t) = \begin{cases} \frac{1}{N} + (1 - \frac{1}{N}) \prod_{s \in \mathbb{T} \cap (0,t)} (1 - N(q-1)s) & \text{if } v_1 = v_2, \\ \frac{1}{N} - \frac{1}{N} \prod_{s \in \mathbb{T} \cap (0,t)} (1 - N(q-1)s) & \text{if } v_1 \neq v_2. \end{cases}$$

5.5. Proof of Proposition 1.1

Proof We begin by reasoning analogously as in [11, Section 6], to deduce that

$$L_{G,v_1} H_{K_N}(v_1, v_2; t) = -e_{-N}(t, t_0) \left\{ \begin{array}{ll} (N-1) - d_G(v_1), & \text{if } v_1 = v_2; \\ -1, & \text{if } v_1 \sim_c v_2; \\ 0, & \text{otherwise} \end{array} \right\} = -e_{-N}(t, t_0) u_G(v_1, v_2).$$

From the expression (5.9) for the heat kernel, we get that

$$(H_{K_N} *_G L_{G,v_1} H_{K_N})(v_1, v_2; t) = -u_G(v_1, v_2) \int_{t_0}^{t} \left(\frac{1}{N} + (1 - \frac{1}{N}) e_{-N}(t, \sigma(s)) \right) e_{-N}(s, t_0) \Delta s$$
$$- \sum_{v \in VG\, v \neq v_1} u_G(v, v_2) \int_{t_0}^{t} \left(\frac{1}{N} - \frac{1}{N} e_{-N}(t, \sigma(s)) \right) e_{-N}(s, t_0) \Delta s.$$

From the definition of $u_G(v, v_2)$ it is immediate that $\sum_{v \in VG} u_G(v, v_2) = 0$; hence,

$$(H_{K_N} *_G L_{G,v_1} H_{K_N})(v_1, v_2; t) = -u_G(v_1, v_2) \int_{t_0}^{t} e_{-N}(t, \sigma(s)) e_{-N}(s, t_0) \Delta s$$
$$= -u_G(v_1, v_2)(e_{-N} * e_{-N})(t).$$

By applying [2, Theorem 5.3], we deduce that

$$(H_{K_N} *_G L_{G,v_1} H_{K_N})(v_1, v_2; t) = -u_G(v_1, v_2) \sum_{\ell=0}^{\infty} (\ell+1)(-N)^{\ell} h_{\ell+1}(t, t_0).$$

Next by reasoning analogously, we can compute $((H_{K_N} *_G L_{G,v_1} H_{K_N}) *_G L_{G,v_1} H_{K_N})(v_1, v_2; t)$ to get that

$$\begin{aligned}(H_{K_N} *_G (L_{G,v_1} H_{K_N})^{*_G 2})(v_1, v_2; t) &= U_G^2(v_1, v_2) \int_{t_0}^{t} \sum_{\ell=0}^{\infty} (\ell+1)(-N)^{\ell} h_{\ell+1}(t, \sigma(s)) e_{-N}(s, t_0) \Delta s \\ &= U_G^2(v_1, v_2) \sum_{\ell=0}^{\infty} \binom{\ell+2}{2} (-N)^{\ell} h_{\ell+2}(t, t_0),\end{aligned}$$

where $U_G^2(v_1, v_2)$ denotes the v_1, v_2 entry of the matrix U_G^2. It is now trivial to deduce for any $k \geq 1$ that

$$(H_{K_N} *_G (L_{G,v_1} H_{K_N})^{*_G k})(v_1, v_2; t) = (-1)^k U_G^k(v_1, v_2) \sum_{\ell=0}^{\infty} \binom{\ell+k}{k} (-N)^{\ell} h_{\ell+k}(t, t_0).$$

When employing Theorem 4.7 with f taken to be H_{K_N}, the proof of Proposition 1.1 is completed. □

Remark 5.5 When $\mathbb{T} = \mathbb{R}$ and $t_0 = 0$, then

$$E_{-N,k}(t) = \sum_{\ell=0}^{\infty} \frac{(\ell+k)!}{\ell! k!} (-N)^{\ell} \frac{t^{\ell+k}}{(\ell+k)!} = e^{-Nt} \cdot \frac{t^k}{k!}.$$

In other words, the statement of Proposition 1.1 reduces to the main result of [11, Section 6] with $B = U_G$.

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References

[1] Bohner M, Cuchta T. The Bessel difference equation. Proceedings of American Mathematical Society 2017; 145 (4): 1567-1580. https://doi.org/10.1090/proc/13416

[2] Bohner M, Guseinov GS. The Convolution on Time Scales. Abstract and applied analysis 2007; Article ID 58373, 24pp. https://doi.org/10.1155/2007/58373

[3] Bohner M, Lutz DA. Asymptotic expansions and analytic dynamic equations. ZAMM - Journal of Applied Mathematics and Mechanics 2006; 86 (1): 37-45. https://doi.org/10.1002/zamm.200410219

[4] Bohner M, Peterson A. Dynamic Equations on Time Scales: An Introduction with Applications. Boston, MA, USA: Birkhüser, 2001.

[5] Campbell J. The SMM model as a boundary value problem using the discrete diffusion equation. Theoretical Population Biology 2007; 72 (4): 539-546. https://doi.org/10.1016/j.tpb.2007.08.001

[6] Cadart C, Venkova L, Recho P, Lagomarsino MC, Piel M. The physics of cell-size regulation across timescales. Nature Physics 2019; 15 (10): 993-1004. https://doi.org/10.1038/s41567-019-0629-y

[7] Cadavid CA, Hoyos P, Jorgenson J, Smajlović L, Vélez JD. On an approach for evaluating certain trigonometric character sums using the discrete time heat kernel. European Journal of Combinatorics 2023; 108, Paper No. 103635, 23 pp. https://doi.org/10.1016/j.ejc.2022.103635

[8] Cadavid CA, Hoyos P, Jorgenson J, Smajlović L, Vélez JD. Discrete diffusion-type equation on regular graphs and its applications. Journal of Difference Equations and Applications 2023; 29 (4): 455-488. https://doi.org/10.1080/10236198.2023.2219784

[9] Cantrell RS, Cosner C, Lewis MA, Lou Y. Evolution of dispersal in spatial population models with multiple timescales. Journal of Mathematical Biology 2018; 80 (1–2): 3–37. https://doi.org/10.1007/s00285-018-1302-2

[10] Chavel I. Eigenvalues in Riemannian Geometry. Academic Press, 1984.

[11] Chinta G, Jorgenson J, Karlsson A, Smajlović L. The parametrix construction of the heat kernel on a graph, arxiv preprint, arXiv:2308.04174, 2023.

[12] Cho S, Kim P, Song R, Vondracek Z. Heat kernel estimates for subordinate Markov processes and their applications. Journal of Differential Equations 2022; 316: 28-93. https://doi.org/10.1016/j.jde.2022.01.044

[13] Cuchta T. Discrete analogues of some classical special functions. PhD, Missouri University of Science and Technology, Rolla, USA, 2015.

[14] Dodziuk J. Elliptic operators on innite graphs, Analysis, geometry and topology of elliptic operators. In: Papers in honor of Krzysztof P. Wojciechowski, World Scientific Publications, Hackensack, NJ, 2006. pp. 353-368.

[15] Dodziuk J, Mathai V. Kato's inequality and asymptotic spectral properties for discrete magnetic Laplacians. In: The ubiquitous heat kernel, Contemporary Mathematics vol.398, American Mathematical Society, Providence, RI, 2006, 69-81.

[16] Hernández-Balaguera E. Numerical approximations on the transient analysis of bioelectric phenomena at long time scales via the Mittag-Leffler function. Chaos, Solitons & Fractals 2021; 145, paper no. 110768. https://doi.org/10.1016/j.chaos.2021.110768

[17] Hilger S. Ein Maßkettenkalkül mit Anwendung auf Zentrumsmannigfaltigkeiten. PhD, Universität Würzburg, Würzburg, Germany, 1988. (in German)

[18] Hilger S. Analysis on measure chains – a unified approach to continuous and discrete calculus. Results in Mathematics 1990; 18: 18-56. https://doi.org/10.1007/BF03323153

[19] Iturria-Medina Y, Sotero RC, Canales-Rodríguez EJ, Alemán-Gómez Y, Melie-García L. Studying the human brain anatomical network via diffusion-weighted MRI and Graph Theory. Neuroimage 2008; 40 (3): 1064-1076.

[20] Jorgenson J, Karlsson A, Smajlović L. Constructing heat kernels on infinite graphs. https://doi.org/10.48550/arXiv.2404.11535

[21] Khan ZA, Arora P. Computational approach of dynamic integral inequalities with applications to timescale calculus. Computational and Applied Mathematics 2020; 39 (4), article no. 273. https://doi.org/10.1007/s40314-020-01323-3

[22] Lang S. Math talks for undergraduates. New York, NY, USA: 1999.

[23] Lin Y, Ngai S-M, Yau S-T. Heat kernels on forms defined on a subgraph of a complete graph. Mathematische Annalen 2021; 380 (3-4): 1891-1931. https://doi.org/10.1007/s00208-021-02215-5

[24] Merkurjev E, Bertozzi AL, Chung F. A semi-supervised heat kernel pagerank MBO algorithm for data classification. Communnications in Mathematical Sciences 2018; 16 (5): 1241-1265. https://dx.doi.org/10.4310/CMS.2018.v16.n5.a4

[25] Minakshisundaram S. Eigenfunctions on Riemannian manifolds. The Journal of the Indian Mathematical Society (New Series) 1953; 17: 159-165.

[26] Minakshisundaram S, Pleijel Å. Some properties of the eigenfunctions of the Laplace-operator on Riemannian manifolds. Canadian Journal of Mathematics 1949; 1: 242-256. https://doi.org/10.4153/CJM-1949-021-5

[27] Piantadosi J, Boland J, Howlett P. Generating synthetic rainfall on various timescales—daily, monthly and yearly. Environmental Modeling & Assessment 2008; 14 (4): 431-438. https://doi.org/10.1007/s10666-008-9157-3

[28] Slavík A. Discrete Bessel functions and partial difference equations. Journal of Difference Equations and Applications 2018; 24 (3): 425-437. https://doi.org/10.1080/10236198.2017.1416107

[29] Slavík A, Stehlík P. Dynamic diffusion-type equations on discrete-space domains. Journal of Mathematical Analysis and Applications 2015; 427: 525-545. https://doi.org/10.1016/j.jmaa.2015.02.056