Constructing heat kernels on infinite graphs *

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Abstract

Let G be an infinite, edge- and vertex-weighted graph with certain reasonable restrictions. We construct the heat kernel of the associated Laplacian using an adaptation of the parametrix approach due to Minakshisundaram-Pleijel in the setting of Riemannian geometry. This is partly motivated by the wish to relate the heat kernels of a graph and a subgraph, or of a domain and a discretization of it. As an application, assuming that the graph is locally finite, we express the heat kernel $H_G(x, y; t)$ as a Taylor series with the lead term being $a(x, y)t^r$, where r is the combinatorial distance between x and y and $a(x, y)$ depends (explicitly) upon edge and vertex weights. In the case G is the regular $(q + 1)$-tree with $q \geq 1$, our construction reproves different explicit formulas due to Chung-Yau and to Chinta-Jorgenson-Karlsson. Assuming uniform boundedness of the combinatorial vertex degree, we show that a dilated Gaussian depending on any distance metric on G, which is uniformly bounded from below can be taken as a parametrix in our construction. Our work extends in part the recent articles [LNY21, CJKS23] in that the graphs are infinite and weighted.

1 Introduction

In the seminal article [MP49], Minakshisundaram and Pleijel established a general method by which one can construct explicitly the heat kernel for the Laplacian operator associated to a smooth compact Riemannian manifold. As stated in [MP49], their method is a generalization of previous work by Carleman. In effect, one begins with an initial approximation for the heat kernel for time approaching zero, called a parametrix H, and then one forms a Neumann series $F(H)$ of convolutions only involving the parametrix H. It is then shown that $H + F(H)$ equals the heat kernel sought. So, in essence, the heat kernel is realized as a type of fixed point theorem since one has some flexibility when choosing the parametrix H.

In this paper we will develop a similar methodology by which one can construct the heat kernel associated to the graph Laplacian for a rather general infinite graph X. Our approach is most directly inspired by [Mi49] and [Mi53] as well as [Ro83] and [Ch84]. The results of this paper extend results from [CJKS23] in which a parametrix construction is carried out for finite graphs whose vertex weight function is identically equal to one, compare also with [LNY21, section 5]. Moreover, our results complements those from [Wo09] where the heat kernel on infinite graphs is constructed by exhausting the infinite graph with finite, connected subgraphs.

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One motivation for undertaking this study is the following. Some of the most significant applications of heat kernel analysis (see [JoLa01, Gr09] and references therein) come from relating the heat kernels on two spaces X and Y via a quotient structure $Y \twoheadrightarrow X$, such as Poisson summation, Jacobi theta inversion and other trace formulas. The parametrix construction can naturally be used to instead set up a comparison in a subspace situation $X \hookrightarrow Y$. This is the point of view taken by Lin, Ngai and Yau in [LNY21], who wrote that it is useful to express the heat kernel expansions of X, a finite graph, in terms of that of Y, a complete graph containing X. These authors viewed this in analogy with relating the heat kernel on a compact d-dimensional manifold with $\mathbb{R}^d$ as done in Riemannian geometry. In our setting, since our graphs X are infinite, this would rather correspond to non-compact manifolds or open domains in $\mathbb{R}^d$. Note that we also allow our space Y, via the parametrix chosen, to be more general, for example it could be a graph containing X or a domain that X provides a discretization of.

Let G be an infinite connected graph with vertex weights $\theta(x)$ and edge weights w_{xy} satisfying conditions (G1) and (G2') given below. The Laplace operator on functions is

$$\Delta_G f(x) = \frac{1}{\theta(x)} \sum_{y \in VG} (f(x) - f(y)) w_{xy}. \tag{1}$$

See section 2 for all details. The main result of this paper is an explicit construction of the heat kernel on G associated to this Laplacian, starting with a parametrix, see Definition 6 for the definition:

Theorem 1. *Let H be a parametrix of order $k \geq 0$ for the heat operator $L_G = \Delta_G + \partial_t$. For $x, y \in VG$ and $t \in \mathbb{R}_{\geq 0}$, let*

$$F(x, y; t) := \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{G,x} H)^{*\ell}(x, y; t). \tag{2}$$

This series converges absolutely and uniformly on every compact subset of $VG \times VG \times \mathbb{R}_{\geq 0}$. The heat kernel H_G is given by

$$H_G(x, y; t) = H(x, y; t) + (H * F)(x, y; t) \tag{3}$$

and

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

Here, $*$ denotes the convolution of two functions with a domain $VG \times VG \times \mathbb{R}_{\geq 0}$, see Definition 3. Our construction allows for a variety of expressions for the heat kernel, and we focus on two types of parametrix, the simple Dirac delta function (section 5) and more elaborate parametrix coming from distance functions (section 6).

First, we show in section 5 that the Dirac delta function $\frac{1}{\theta(x)} \delta_{x=y}$ on $L^1(\theta)$ can be chosen as a parametrix, under additional assumption that the graph is locally finite, meaning that for each $x \in VG$, the number of vertices adjacent to x is finite. Then, in Proposition 9 below we show that by taking the Dirac delta function as the parametrix in our main theorem, the heat kernel $H_G(x, y; t)$ on G can be expressed as

$$H_G(x, y; t) = \frac{1}{\theta(x)} \delta_{x=y} + \sum_{\ell=1}^{\infty} (-1)^{\ell} \frac{t^{\ell}}{\ell!} \sum_{z_1, \ldots, z_{\ell-1} \in VG} \delta_x(z_1) \delta_{z_1}(z_2) \cdot \ldots \cdot \delta_{z_{\ell-1}}(y), \tag{4}$$

where

$$\delta_x(y) := \frac{1}{\theta(x)} \begin{cases} \mu(x), & x = y; \\ -w_{xy}, & x \sim y \\ 0, & \text{otherwise,} \end{cases} \qquad x, y \in VG. \tag{5}$$

The combinatorial expression (4) for the heat kernel further highlights the local nature of the heat diffusion. Specifically, the first $r+1$ terms in the expansion on the right-hand side of (4) in powers of t depend only on points that are at combinatorial distance at most r from the starting point x. Moreover, if the combinatorial distance $d(x,y)$ between x and y is $r \geq 2$, then $\delta_x(z_1)\delta_{z_1}(z_2)\cdot \ldots \cdot \delta_{z_{\ell-1}}(y) = 0$ for any choice $z_1, \ldots, z_{\ell-1} \in VG$ of $\ell - 1 \leq r-1$ points which yields the following corollary.

Corollary 2. *Let G be an infinite weighted, connected and locally finite graph satisfying conditions (G1) and (G2'). Then, for all $x, y \in VG$ with the combinatorial distance $d(x,y) = r \geq 1$ and all $t > 0$ we have*

$$\left| H_G(x,y;t) - (-1)^r \frac{t^r}{r!} c_r(x,y) \right| \leq t^{r+1} C(x,y;t),$$

where $c_r(x,y) = \sum_{z_1,\ldots,z_{r-1} \in VG} \delta_x(z_1)\delta_{z_1}(z_2)\cdot \ldots \cdot \delta_{z_{r-1}}(y)$ and

$$C(x,y;t) = \left| \sum_{\ell=r+1}^{\infty} (-1)^{\ell} \frac{t^{\ell-r-1}}{\ell!} \sum_{z_1,\ldots,z_{\ell-1} \in VG} \delta_x(z_1)\delta_{z_1}(z_2)\cdot \ldots \cdot \delta_{z_{\ell-1}}(y) \right|$$

is bounded as $t \downarrow 0$.

Therefore, the heat kernel $H_G(x,y;t)$, for small time t is asymptotically equal $\frac{(-1)^r}{r!} c_r(x,y) t^r$. This was proved in [KLMST16, Theorem 2.2.], with the constant multiplying t^r and the upper bound $C(x,y;t)$ expressed in a different way.

Second, in section 6 we consider a parametrix which is inspired by the Gaussian as the heat kernel on $\mathbb{R}$ (see [Gr09], section 9 for generalizations and modifications in higher-dimensional setting). Namely, in Proposition 12 below we show that, assuming uniform boundedness of combinatorial vertex degree, for *any* distance metric d on G such that $d(x,y) \geq \delta > 0$ for all distinct points $x, y \in VG$, the function $H_d : VG \times VG \times [0,\infty) \to [0,\infty)$, defined as

$$H_d(x,y;t) := \frac{1}{\sqrt{\theta(x)\theta(y)}} \exp(-(\theta(x)\theta(y)d^2(x,y))/t) \text{ with } H_d(x,y;0) = \lim_{t \downarrow 0} H_d(x,y;t)$$

can be taken as a parametrix in our construction of the heat kernel.

There has been extensive studies of heat kernels within the field of spectral graph theory. However, as noted in [LNY21], there are few instances of explicit evaluations of heat kernels on infinite graphs. The main examples are lattice graphs (see [CY97, Be03, KN06]) and regular trees (see [CY99] and [CJK15]). These formulas will be rederived below from the general methodology we develop in this article (see Example 11). For instance, let G be a $(q+1)$-regular tree, which has special significance since it is the universal covering of every $(q+1)$-regular graph, then we have

$$H_G(x,y;t) = q^{-r/2} e^{-(q+1)t} I_r(2\sqrt{q}t) - (q-1)e^{-(q+1)t} \sum_{j=1}^{\infty} q^{-(r+2j)/2} I_{2j+r}(2\sqrt{q}t). \tag{6}$$

where $I_n(t)$ is the classical I-Bessel function. This is the formula in [CJK15].

As already mentioned, comparing different heat kernel expressions often leads to significant consequences. In the graph setting, we can refer to recent articles [GLY22], [CHJSV23] and [JKS23] that use the heat kernel on the lattice graph and its quotient to obtain explicit evaluations of trigonometric sums. See also [HSSS23] for series identities of I-Bessel functions, from which the authors deduce transformation formulas for the Dedekind eta-function.

By choosing a different metric on G, and a few examples are presented in section 6.1 below, we get different "seeds" H_d in the parametrix construction. Given that in our setting the heat kernel is unique, when equating the expressions for the heat kernels constructed using H_d with different distances d yields many new identities. Going further, when taking the Laplace transform of such identities may be particularly useful since the Laplace transform of a time convolution of two functions equals the product of Laplace transforms.

When the Laplacian extends to a bounded, self-adjoint operator on $L^2(\theta)$, the heat kernel possesses a spectral expansion in terms of the eigenvalues and the eigenfunctions of the Laplacian. As such, when using the parametrix construction of the heat kernel and starting with the seed H_d, which is of a geometric nature, one can also deduce identities relating the sum over the eigenvalues to the length spectrum of the graph. This, in turn, may serve as a starting point for deducing trace-type formulas, see for example [CY97], [TW03], [HNT06] or [Mn07]. A similar argument in the setting of compact hyperbolic Riemann surfaces yields a succinct proof of the Selberg trace formula; see Remark 3.3 of [GJ18].

1.1 Organization of the paper

This paper is organized as follows. We start in section 2 by describing the assumptions on the graph G, followed by section 3 where we define the convolution on the space $L^p(\theta)$ and prove some of its properties, which ensure that a certain convolution series is convergent. In section 4 we define the notion of a parametrix and prove our main theorem, Theorem 8, which computes the heat kernel by starting with a parametrix. We then proceed by constructing different parametrix and their associated heat kernels. In section 5 it is proved that the Dirac delta on $L^1(\theta)$ can be taken as the parametrix, under the assumption that the graph G is locally finite. In section 6 we develop further examples, under assumption that the combinatorial vertex degree is uniformly bounded on G. In particular, we show that the function H_d defined above can be taken as a parametrix for an arbitrary choice of metric d on G provided d is uniformly bounded from below. We conclude the paper with several remarks and questions for further studies.

2 Our setup

Let G be a countably infinite, vertex-weighted, edge-weighted, and connected graph with the vertex set VG. The vertex weights are defined by the function $\theta : VG \to (0, \infty)$ with full support, meaning $\theta(x) > 0$ for all $x \in VG$. The edge weights are defined by a nonnegative function $w : VG \times VG \to [0, \infty)$, and we shall use the notation $w_{xy} = w(x, y)$. We assume that w is symmetric, meaning that $w_{xy} = w_{yx}$ for all $x, y \in VG$, hence the graph is undirected. If $w_{xy} = 0$ we say there is no edge between the vertices x and y. When $w_{xy} > 0$, the vertices x and y are said to be adjacent or neighbors, and we write $x \sim y$. Furthermore, we assume that $w_{xx} = 0$ for all x, meaning that G has no loops. We refer to [Fo13] p. 117 as well as [Fo14] for an interesting probabilistic interpretation of the edge weights and the vertex weights.

Let $p \in [1, \infty]$ be a real number or $+\infty$, and let $L^p(\theta)$ denote the classical L^p space of functions on VG with respect to the pointwise vertex measure θ. Specifically, the function

$f : VG \to \mathbb{C}$ belongs to $L^p(\theta)$ for $p \in (1, \infty)$ if and only if

$$\sum_{x \in VG} |f(x)|^p \theta(x) < \infty.$$

Since θ has a full support, any $f \in L^\infty(\theta)$ is such that f is uniformly bounded on VG. We denote by $\|f\|_{p,\theta}$ the L^p-norm of f. When $p = 2$, the space $L^2(\theta)$ is a Hilbert space with the inner product

$$\langle f, g \rangle_\theta := \sum_{x \in VG} f(x)\overline{g(x)}\theta(x).$$

Following [KL12], we define the Laplace operator Δ_G acting on functions $f : VG \to \mathbb{C}$ by

$$\Delta_G f(x) = \frac{1}{\theta(x)} \sum_{y \in VG} (f(x) - f(y)) w_{xy}. \tag{7}$$

The natural domain of definition is $\mathcal{D}(\Delta_G) := \{f \in L^2(\theta) : \Delta_G f \in L^2(\theta)\}$.

For any $x \in VG$, define

$$\mu(x) := \sum_{y:\, x \sim y} w_{xy}.$$

For us, we will assume throughout this paper that θ need not equal μ. In general, the Laplacian Δ_G is not bounded, nor possesses a unique self-adjoint extension. For this reason, different authors imposed the following assumptions on the (infinite) graph G.

(G1) **Uniform boundedness of the weighted degree.** There exists a positive constant M such that for all $x \in VG$ we have that

$$\mu(x) := \sum_{y:\, x \sim y} w_{xy} \le M.$$

(G2) **Unbound sum for the vertex weights.**

$$\sum_{x \in VG} \theta(x) = \infty.$$

The assumptions (G1) and (G2) imply that Δ_G with domain $\mathcal{D}(\Delta_G)$ is self-adjoint; see [KL12, Theorem 5]. Yet, Δ_G is not necessarily bounded operator on $L^2(\theta)$. The operator Δ_G is bounded on $L^2(\theta)$ if and only if

$$A(G, w, \theta) := \sup_{x \in VG} \frac{\mu(x)}{\theta(x)} < \infty, \tag{8}$$

see page 66 of [Da93], [HKLW12] or [KLW21, Theorem 1.27]. In view of this, throughout this paper we will replace (G2) with the following condition on the vertex weight function

(G2') **Uniform lower bound for the vertex weights.** There exists $\eta > 0$ such that

$$\inf_{x \in VG} \theta(x) > \eta.$$

Condition (G2') arises naturally in [Fo14]. Conditions (G1) and (G2') ensure that Δ_G extends to a bounded operator on $L^2(\theta)$ which is, according to [KL12, Theorem 6], essentially self-adjoint on the set of compactly supported functions (with the maximal associated Dirichlet form). Essential self-adjointness means that the operator possesses a unique self-adjoint extension.

Throghout this paper, the weighted graph G satisfies conditions (G1) *and* (G2').

The *heat kernel* on the graph G associated to the weighted graph Laplacian $\Delta_{G,x}$, when acting on functions in the variable x, is the unique solution $H_G(x,y;t)$ to the differential equation

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

with the property that

$$\lim_{t\to 0} H_G(x,y;t) = \frac{1}{\theta(x)}\delta_{x=y} = \begin{cases} \frac{1}{\theta(x)}, & \text{if } x = y \\ 0, & \text{if } x \neq y \end{cases}, \tag{9}$$

where δ is the Kronecker delta function.

For the proof of the existence and uniqueness of the heat kernel on G, we refer to [Do84], [DM06] for the case when $\theta(x) \equiv 1$ and to [Hu12], in a general setting. Let us note that the uniqueness essentially follows from the fact that (G1) and (G2') imply that Δ_G is stochastically complete; see [Wo21, Theorem 4.3] as well as the extensive bibliography therein. Specifically, according to [Wo21, Theorem 3.3], stochastic completeness is equivalent to unique dependence of the bounded solution to the heat equation from its initial condition which are given by a bounded function on G.

3 Convolution on $L^p(\theta)$

For any $p \in [1,\infty]$ we denote by q its conjugate, meaning the number $q \in [1,\infty]$ such that $\frac{1}{p} + \frac{1}{q} = 1$, or $p = 1$ if $q = \infty$. Let us start by defining the convolution of two functions that belong to conjugate $L^p(\theta)$ spaces.

Definition 3. With the notation as above, let $F_1, F_2 : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$ be two functions such that for any $t > 0$, those functions, when viewed as functions on $VG \times VG$, belong to $L^p(\theta)$ in the second variable and $L^q(\theta)$ in the first variable, respectively. Assume further that for all $b > 0$ and for all $x, y \in VG$, the function $\langle F_1(x,\cdot;t-r), F_2(\cdot,y;r)\rangle_\theta$, which is well defined, due to the Hölder inequality, is integrable on $[0,b]$. The *convolution* of functions F_1 and F_2 is defined to be

$$\begin{aligned}(F_1 * F_2)(x,y;t) &:= \int_0^t \langle F_1(x,\cdot;t-r), F_2(\cdot,y;r)\rangle_\theta dr \\ &= \int_0^t \sum_{z\in VG} F_1(x,z,t-r)F_2(z,y;r)\theta(z)dr. \end{aligned}\tag{10}$$

The above convolution is not commutative in general but it is associative, under suitable assumptions on functions convolved. We have the following lemma.

Lemma 4. *Let $F_1, F_2 : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$ be as in Definition 3. 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 all $x, y \in VG$, we have*

$$\|F_1(x,\cdot;t)\|_{p,\theta} \leq C_1 t^k \quad \text{and} \quad \|F_2(\cdot,y;t)\|_{q,\theta} \leq C_2 t^\ell.$$

Then, for all $x, y \in VG$ we have

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

Proof. From the Hölder inequality we get

$$\begin{aligned} |(F_1 * F_2)(x,y;t)| &\leq \int_0^t \|F_1(x,\cdot;t-r)\|_{p,\theta} \|F_2(\cdot,y;r)\|_{q,\theta} \, dr \\ &\leq C_1 C_2 \int_0^t r^k (t-r)^\ell \, dr = C_1 C_2 \frac{k!\ell! t^{k+\ell+1}}{(k+\ell+1)!}, \end{aligned}$$

as claimed. □

Let $f = f(x,y;t) : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$ be a function with the following property. For any $T > 0$, for all $t \in (0,T]$, and all arbitrary, but fixed, $x, y \in VG$ the functions $f(\cdot,y;t) : VG \to \mathbb{R}$ and $f(x,\cdot;t) : VG \to \mathbb{R}$ belong to $L^p(\theta) \cap L^q(\theta)$ and the function $f(x,y;\cdot) : (0,T] \to \mathbb{R}$ is integrable. For any positive integer ℓ and any such function f, we can inductively define the ℓ-fold convolution $(f)^{*\ell}(x,y;t)$ for $t \in (0,T]$ by setting $(f)^{*1}(x,y;t) = f(x,y;t)$ and, for $\ell \geq 2$ we put

$$(f)^{*\ell}(x,y;t) := \left(f * (f)^{*(\ell-1)}\right)(x,y;t),$$

under additional assumption that $(f)^{*(\ell-1)}(x,\cdot;t) \in L^q(\theta)$ for all $t \in (0,T]$ and all $\ell \geq 2$.

With this notation we have the following lemma.

Lemma 5. *Let $f = f(x,y;t) : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$. Assume that for all $x, y \in VG$ and all $t_0 \in \mathbb{R}_{>0}$, the function $f(x,y;\cdot)$ is integrable on the interval $(0,t_0]$ and $f(x,\cdot;t) \in L^1(\theta)$ for all $t \in (0,t_0]$. Assume further that for all $t_0 \in \mathbb{R}_{>0}$ there exists a constant C, depending only upon t_0, and integer $k \geq 0$ such that*

$$|f(x,y;t)| \leq Ct^k \quad \text{for all } x, y \in VG \text{ and } 0 < t < t_0.$$

Then the series

$$\sum_{\ell=1}^{\infty} (-1)^\ell (f)^{*\ell}(x,y;t) \tag{11}$$

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

$$\left(f * \left(\sum_{\ell=1}^{\infty} (-1)^\ell (f)^{*\ell}\right)\right)(x,y;t) = \sum_{\ell=1}^{\infty} (-1)^\ell (f)^{*(\ell+1)}(x,y;t). \tag{12}$$

and

$$\sum_{\ell=1}^{\infty} \left|(f)^{*\ell}(x,y;t)\right| = O(t^k) \quad \text{as } t \to 0, \tag{13}$$

where the implied constant is independent of $x, y \in VG$.

Proof. Let A be an arbitrary compact subset of $VG \times VG \times \mathbb{R}_{>0}$. Let $t_0 > 0$ be such that $A \subseteq VG \times VG \times (0,t_0]$. We apply Lemma 4, with $p = \infty$, $q = 1$ to get that

$$|(f * f)(x,y;t)| \leq C\|f\|_{1,\theta} \frac{t^{k+1}}{(k+1)!}, \quad \text{for all } x, y \in VG \text{ and } 0 < t < t_0. \tag{14}$$

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

$$\left|(f^{*(\ell)})(x,y;t)\right| \leq C\|f\|_{1,\theta}^{\ell-1}\frac{t^{k+\ell-1}}{(k+\ell-1)!}, \quad \text{for all } x,y \in VG \text{ and } 0<t<t_0. \tag{15}$$

The assertion regarding the convergence of (11) now follows from the Weierstrass criterion and the fact that $A \subseteq VG \times VG \times (0,t_0]$.

Fix $t>0$. The series (11) converges absolutely. When viewed as a function of y, for any arbitrary but fixed x and for any $0<t<t_0$, the series belongs to $L^\infty(\theta)$. Therefore,

$$\left(f * \left(\sum_{\ell=1}^{\infty}(-1)^\ell (f)^{*\ell}\right)\right)(x,y;t) = \int_0^t \sum_{z\in VG} f(x,z;t-r)\left(\sum_{\ell=1}^{\infty}(-1)^\ell (f)^{*\ell}(z,y;r)\right)\theta(z)dr. \tag{16}$$

From the bound (15), combined with the Hölder inequality with $p=1$, $q=\infty$ we have, for an arbitrary $t\in(0,t_0)$ and $0<r<t$ that

$$\sum_{\ell=1}^{\infty}\sum_{z\in VG}\left|f(x,z;t-r)(f)^{*\ell}(z,y;r)\right|\theta(z) \leq C\|f\|_{1,\theta}t^k \exp(t\|f\|_{1,\theta}).$$

Hence we may interchange the sum over ℓ with the sum over $z\in VG$ in (16). Reasoning analogously, one easily shows that we may interchange the infinite sum over ℓ with the integral from 0 to t, to deduce that

$$\left(f * \left(\sum_{\ell=1}^{\infty}(-1)^\ell (f)^{*\ell}\right)\right)(x,y;t) = \sum_{\ell=1}^{\infty}(-1)^\ell \int_0^t \sum_{z\in VG} f(x,z;t-r)(f)^{*\ell}(z,y;r)\theta(z)dr,$$

which proves (12).

Finally, the bound (15) and the fact that the series (11) converges absolutely on $VG\times VG\times(0,t_0]$ yield that

$$\sum_{\ell=1}^{\infty}\left|(f)^{*\ell}(x,y;t)\right| \leq C\|f\|_{1,\theta}t^k\exp(t\|f\|_{1,\theta}),$$

which proves (13). □

4 The parametrix construction of the heat kernel on G

The heat operator L_G on the graph G is defined by

$$L_G = \Delta_G + \frac{\partial}{\partial t}. \tag{17}$$

With this notation, 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

$$L_{G,x}H_G(x,y;t)=0$$

satisfying the initial condition (9). The subscript x on L_x indicates the sum (7) which defines the Laplacian is over neighbors of x, the first space variable.

Definition 6. Let $k \geq 0$ be an integer. A *parametrix* H order k for the heat operator L_G on G is any continuous function $H = H(x, y; t) : VG \times VG \times [0, \infty)$ which is smooth in time variable t, integrable in each space variable, and satisfies the following properties.

1. For all $x, y \in VG$,
$$H(x, y; 0) = \lim_{t \to 0} H(x, y; t) = \frac{1}{\theta(x)} \delta_{x=y}. \tag{18}$$

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

3. For all $x \in VG$, $t > 0$ we have that $\Delta_{G,x} H(x, \cdot; t)$ and $\frac{\partial}{\partial t} H(x, \cdot; t)$ are in $L^1(\theta)$.

4. For any $t_0 > 0$ there exists a constant $C = C(t_0)$, depending only on t_0, such that
$$|L_{G,x} H(x, y; t)| \leq C(t_0) t^k \quad \text{for } t \in (0, t_0] \text{ and all } x, y \in VG.$$

Note that the third assumption on the parametrix H implies that $L_{G,x} H(x, \cdot; t) \in L^1(\theta)$.

Lemma 7. *Let H be a parametrix for the heat operator on G of any order. Let $f = f(x, y; t) : VG \times VG \times \mathbb{R}_{>0} \to \mathbb{R}$ be a continuous function in t for all $x, y \in VG$. Assume further that for all $t > 0$ the function $f(x, y; t)$ when viewed as a function on $VG \times VG$ is uniformly bounded. Then*
$$L_{G,x}(H * f)(x, y; t) = f(x, y; t) + (L_{G,x} H * f)(x, y; t)$$
for all $x, y \in VG$ and $t \in \mathbb{R}_{>0}$.

Proof. As stated $f(\cdot, y; t) \in L^\infty(\theta)$ and $H(x, \cdot; t), \Delta_{G,x} H(x, \cdot; t) \in L^1(\theta)$ for all $(x, y; t) \in VG \times VG \times (0, \infty)$. Therefore, the convolutions $H * f$ and $(\Delta_{G,x} H) * f$ are well defined, and we have that
$$\begin{aligned} L_{G,x}(H * f)(x, y; t) &= \frac{\partial}{\partial t}(H * f)(x, y; t) + \Delta_{G,x}(H * f)(x, y; t) \\ &= \frac{\partial}{\partial t}(H * f)(x, y; t) + ((\Delta_{G,x} H) * f)(x, y; t), \end{aligned} \tag{19}$$
where the second equation follows from the fact that the Laplacian acts on the first variable only.

The function $\sum_{z \in VG} H(x, z; t - r) f(z, y; r) \theta(z)$ is continuous in the time variable, so we can apply the Leibniz integration formula. Upon doing so, we obtain that the first term on the right hand side of (19) is equal to
$$\frac{\partial}{\partial t} \int_0^t \sum_{z \in VG} H(x, z; t - r) f(z, y; r) \theta(z) dr \tag{20}$$
$$= \sum_{z \in VG} H(x, z; 0) f(z, y; t) \theta(z) + \int_0^t \frac{\partial}{\partial t} \sum_{z \in VG} H(x, z; t - r) f(z, y; r) \theta(z) dr.$$

The assumptions that f is uniformly bounded and that $\frac{\partial}{\partial t} H(x, \cdot; t) \in L^1(\theta)$ combine to yield that
$$\frac{\partial}{\partial t} \sum_{z \in VG} H(x, z; t - r) f(z, y; r) \theta(z) = \sum_{z \in VG} \frac{\partial}{\partial t} H(x, z; t - r) f(z, y; r) \theta(z).$$

Given that $H(x,z;0)=0$ unless $x=z$, we get from (20) that

$$\frac{\partial}{\partial t}\int\limits_0^t \sum_{z\in VG} H(x,z;t-r)f(z,y;r)\theta(z)dr = f(x,y;t) + \left(\frac{\partial}{\partial t}H * f\right)(x,y;t).$$

Therefore,

$$\begin{aligned} L_{G,x}(H*f)(x,y;t) &= \frac{\partial}{\partial t}(H*f)(x,y;t) + (\Delta_{G,x}H*f)(x,y;t) \\ &= f(x,y;t) + \left(\frac{\partial}{\partial t}H*f\right)(x,y;t) + (\Delta_{G,x}H*f)(x,y;t) \\ &= f(x,y;t) + (L_{G,x}H*f)(x,y;t), \end{aligned}$$

as claimed. □

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

Theorem 8. *Let H be a parametrix of order $k \geq 0$ for the heat operator on G. For $x,y\in VG$ and $t\in\mathbb{R}_{\geq 0}$, let*

$$F(x,y;t) := \sum_{\ell=1}^{\infty}(-1)^{\ell}(L_{G,x}H)^{*\ell}(x,y;t). \tag{21}$$

Then the Neumann series (21) *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 $\Delta_{G,x}$ is given by*

$$H_G(x,y;t) = H(x,y;t) + (H*F)(x,y;t) \tag{22}$$

and

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

Proof. Set

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

We want to show that

$$L_{G,x}\tilde{H}(x,y;t) = 0 \quad \text{and} \quad \lim_{t\to 0}\tilde{H}(x,y,t) = \frac{1}{\theta(x)}\delta_{x=y}. \tag{23}$$

By Lemma 5, the series $F(x,y;t)$ defined in (21) converges uniformly and absolutely and has order $O(t^k)$ as $t\to 0$. Since H is in $L^1(\theta)$, Lemma 4 then yields the asymptotic bound that

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

Therefore,

$$\lim_{t\to 0}\widetilde{H}(x,y;t) = \lim_{t\to 0}H(x,y;t) = \frac{1}{\theta(x)}\delta_{x=y}.$$

It remains to prove the vanishing of $L_{G,x}\tilde{H}$ in (23). For this, we can apply Lemma 7 to get that

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

To be precise, in the above calculations we used that absolute convergence of the series defining $F(x,y;t)$ in order to change the order of summation. This completes the proof. □

5 Dirac delta as a parametrix

In (22), the function $H(x,y;t)$ 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. However, the edge data is essential in the definition of the Laplacian, which is used in the construction of the series (21) through the heat operator. In this section we highlight the role of the edge data in the construction.

We assume that an infinite graph G satisfies assumptions (G1), (G2') and the following additional assumption (meaning that the graph is locally finite).

(G3) **Finiteness of the combinatorial vertex degree.** For all $x \in VG$ the number of $y \in VG$ such that $w_{xy} > 0$ is finite.

We have the following proposition.

Proposition 9. *Let G be a connected, undirected infinite graph satisfying assumptions (G1), (G2') and (G3) above. Let $H(x,y;t)$ be a function on $VG \times VG \times [0,\infty)$ defined for all $x, y \in VG$ and all $t \in [0,\infty)$ by*

$$
H(x,y;t) := \frac{1}{\theta(x)}\delta_{x=y}. \tag{24}
$$

Let $\delta_x(y)$ be defined as in (5)*. Then, $H(x,y;t)$ defined by* (24) *is the parametrix of order $k = 0$, and the heat kernel H_G constructed when using* (24) *as a parametrix is given by* (4)*.*

Proof. The set VG is discrete, so then $H(x,y;t)$ is continuous on $VG \times VG \times [0,\infty)$ and smooth in t for fixed x and y. It is evident that H belongs to $L^1(\theta)$ in both space variables and, furthermore, satisfies the initial condition (9). Trivially,

$$
L_{G,x}H(x,y;t) = \Delta_{G,x}H(x,y;t) = \frac{1}{\theta^2(x)}\begin{cases} \mu(x), & x = y; \\ -w_{xy}, & x \sim y \\ 0, & \text{otherwise.} \end{cases} \tag{25}
$$

The function (25) is continuous on $VG \times VG \times [0,\infty)$, hence the second condition for the parametrix in Definition 6 is fulfilled. Moreover, $\Delta_{G,x}H(x,\cdot;t) \in L^1(\theta)$ because the sum

$$
\sum_{z \in VG} \theta(z)\Delta_{G,x}H(x,z;t)
$$

is a finite sum, by the assumption (G3). Since $\frac{\partial}{\partial t}H(x,\cdot;t) \equiv 0$, we conclude that the third condition for the parametrix is fulfilled. Finally, from (25) it is evident that for all $x, y \in VG$ and all $t > 0$ we have

$$|L_{G,x}H(x,y;t)| \leq \frac{\mu(x)}{\theta^2(x)} \leq \frac{M}{\eta^2}.$$

Therefore, $H(x,y;t)$ is a parametrix of order $k = 0$.

The heat kernel, as constructed in Theorem 8 when using the parametrix H, is given by

$$H_G(x,y;t) = H(x,y;t) + \sum_{\ell=1}^{\infty}(-1)^{\ell}\left(H * (L_{G,x}H)^{*\ell}\right)(x,y;t) \tag{26}$$

We have the following evaluation of the first few terms in the convolution series (26). First,

$$\begin{aligned}(H * L_{G,x}H)(x,y;t) &= \int_0^t \sum_{z\in VG} \theta(z)H(x,z;t-\tau)L_{G,z}H(z,y;\tau)d\tau = t\theta(x)\frac{\delta_x(y)}{\theta(x)} \\ &= t\delta_x(y).\end{aligned}$$

Using that $\theta(z)L_{G,z}H(z,y;\tau) = \delta_z(y)$ we get

$$\begin{aligned}(H * L_{G,x}H) * L_{G,x}H(x,y;t) &= \int_0^t \sum_{z\in VG} \theta(z)(t-\tau)\delta_x(z)L_{G,z}H(z,y;\tau)d\tau \\ &= \frac{t^2}{2}\sum_{z\in VG}\delta_x(z)\delta_z(y).\end{aligned}$$

Next, when proceeding by induction, we deduce that

$$\left(H * (L_{G,x}H)^{*\ell}\right)(x,y;t) = \frac{t^{\ell}}{\ell!}\sum_{z_1,\ldots,z_{\ell-1}\in VG}\delta_x(z_1)\delta_{z_1}(z_2)\cdot\ldots\cdot\delta_{z_{\ell-1}}(y).$$

The sum on the right-hand side is finite, since $\delta_x(y)$ is supported on a finite set, due to (G3).

With all this, we conclude that the heat kernel on G is given by (4). □

Example 10. Consider the case when $G = \mathbb{Z}$, meaning the graph whose set of vertices is the set of integers. The two vertices $x, y \in \mathbb{Z}$ are connected if and only if $x - y \in \{-1, 1\}$. For every $x \in G$, let the vertex weight be $\theta(x) = 1$, and assume all edges weights are also equal to one. Let us use (4) to compute the heat kernel on $\mathbb{Z}$.

The product $\delta_x(z_1)\delta_{z_1}(z_2)\cdot\ldots\cdot\delta_{z_{\ell-1}}(y)$ in (4) is non-zero precisely when the sequence $x = z_0, z_1, \ldots, z_{\ell-1}, y = z_\ell \in \mathbb{Z}$ is such that $z_h - z_{h-1} \in \{-1, 0, 1\}$ for all $h = 1, \ldots, \ell$. Such a sequence can be identified with an ℓ-tuple $(a_1, \ldots, a_\ell)$ where $a_1, \ldots, a_\ell \in \{-1, 0, 1\}$.

For $x, y \in \mathbb{Z}$, let $j \geq 0$ be such that $x - y = j$; we will comment later when $x - y = -j$. Then the ℓ-tuple $(a_1, \ldots, a_\ell)$ must have exactly j places all with the values 1. Assume that $k \geq 0$ is the number of places a_h in the ℓ-tuple $(a_1, \ldots, a_\ell)$ which are equal to zero. Then at the remaining $\ell - j - k$ places there must be the same number of entries with 1 and with -1; in particular, k must be such that $\ell - j - k$ is an even number, say i, so we have that $\ell - j - k = 2i$.

Therefore, every ℓ-tuple $(a_1, \ldots, a_\ell)$ corresponding to the sequence $x = z_0, z_1, \ldots, z_{\ell-1}, y = z_\ell \in \mathbb{Z}$ such that $z_h - z_{h-1} \in \{-1, 0, 1\}$ and such that $x - y = j$ is uniquely determined by k

places at which there are zeros, where k is such that $\ell - k - j$ is even, and by $i = \frac{1}{2}(\ell - k - j)$ places at which there are the numbers -1. The remaining places all have the value 1. The number of all such ℓ-tuples of elements from $\{-1, 0, 1\}$ is exactly

$$\binom{\ell}{k}\binom{\ell-k}{i} = \frac{\ell!}{k!i!(\ell-k-i)!},$$

where $\ell = k + j + 2i$. For each such ℓ-tuple, we have

$$\delta_x(z_1)\delta_{z_1}(z_2)\cdot \ldots \cdot \delta_{z_{\ell-1}}(y) = 2^k \cdot (-1)^j = (-1)^{\ell+k}2^k,$$

where the last equality follows since $\ell - k - j$ is even, so $(-1)^j = (-1)^{\ell-k} = (-1)^{\ell+k}$. Therefore, for $x - y = j \geq 0$

$$\sum_{z_1,\ldots,z_{\ell-1}\in VG} \delta_x(z_1)\delta_{z_1}(z_2)\cdot \ldots \cdot \delta_{z_{\ell-1}}(y) = \sum_{\substack{i,k\geq 0 \ k+j+2i=\ell \\ \ell-k-j \text{ even}}} (-1)^{\ell+k}\frac{\ell!}{k!i!(i+j)!}2^k.$$

Finally, we get that

$$\begin{aligned} H_{\mathbb{Z}}(x,y;t) &= \sum_{\ell=0}^{\infty} t^\ell \sum_{\substack{i,k\geq 0 \ k+j+2i=\ell \\ \ell-k-j \text{ even}}} \frac{1}{k!i!(j+i)!}(-2)^k \\ &= \sum_{k=0}^{\infty}\frac{(-2t)^k}{k!}\cdot\sum_{i=0}^{\infty}\frac{t^{j+2i}}{i!(j+i)!} = e^{-2t}I_j(2t), \end{aligned}$$

where $I_j(2t)$ is the I-Bessel function, see [GR07], formula 8.445 with $\nu = j$.

In the case $x - y = -j$, we reverse the roles of 1 and -1 in the above combinatorial argument, we get that $H_{\mathbb{Z}}(x,y;t) = e^{-2t}I_j(2t)$. In summary, we have shown that from (4) one gets that the heat kernel on $\mathbb{Z}$ is $H_{\mathbb{Z}}(x,y;t) = e^{-2t}I_{|x-y|}(2t)$, which was previously established in Bednarchak's thesis or essentially already in [Fe71, p. 60], see also [CY97, Be03, KN06].

Example 11. For $q \geq 2$, let $G = T_{q+1}$ be a $q+1$-regular tree with vertex weights $\theta \equiv 1$. Each vertex is connected to $q+1$ vertices with edges, and we assume the edge weights are all equal to 1. Then $\delta_x(z) = (q+1)$ if $z = x$, $\delta_x(z) = -1$ for the $q+1$ vertices z adjacent to x and $\delta_x(z) = 0$ otherwise. We note that the case $q = 1$ is considered in the previous example. Let us use (4) to compute the heat kernel on T_{q+1}.

The product $\delta_x(z_1)\delta_{z_1}(z_2)\cdot\ldots\cdot\delta_{z_{\ell-1}}(y)$ is non-zero if and only if $x = z_0, z_1, \ldots, z_{\ell-1}, y = z_\ell$ are such that each pair of neighbouring entries are either equal or adjacent. Let $x, y \in T_{q+1}$ be such that their distance is $r \geq 0$. If $\ell \leq r$, the product is obviously zero, so we may assume that $\ell \geq r$.

For any integer j with $0 \leq j \leq \ell - r$, let us assume that exactly j of the ℓ values $\delta_{z_i}(z_{i+1})$ are equal to $(q+1)$. Those values can be chosen in $\binom{\ell}{j}$ ways. For such selection of j points $z_i = z_{i+1}$, the sequence $x = z_0, z_1, \ldots, z_{\ell-1}, y = z_\ell$ becomes a walk of length $\ell - j$ from x to y. Let us denote the number of such walks by $b_{\ell-j}(r)$. Note that he number of walks depends only on the distance r between x and y. Therefore, when including the values taken by $\delta_x(z)$, we get that

$$\begin{aligned} a_\ell(r) = \sum_{z_1,\ldots,z_{\ell-1}\in VG} \delta_x(z_1)\delta_{z_1}(z_2)\cdot\ldots\cdot\delta_{z_{\ell-1}}(x) &= \sum_{j=0}^{\ell-r}\binom{\ell}{j}(q+1)^j(-1)^{\ell-j}b_{\ell-j}(r) \\ = \sum_{j=r}^{\ell}\binom{\ell}{\ell-j}(q+1)^{\ell-j}(-1)^j b_j(r) &= (q+1)^\ell\sum_{j=0}^{\ell}\binom{\ell}{j}(q+1)^{-j}(-1)^j b_j(r). \end{aligned}$$

In the last term, we have adopted the convention that the number of walks of length $j < r$ between two points at distance r to be equal to zero. Therefore,

$$(-1)^\ell a_\ell(r) = \sum_{j=0}^{\ell} \binom{\ell}{j} (-(q+1))^{\ell-j} b_j(r),$$

so then we have that

$$H_{T_{q+1}}(x,y;t) = e^{-(q+1)t} \sum_{k=0}^{\infty} b_k(r) \frac{t^k}{k!}.$$

Let us further evaluate this expression.

The ordinary generating function for the number of walks $b_k(r)$ of length k on the $(q+1)$-regular tree, between two points at a distance r is given by

$$f_{q+1}(t) = \frac{2q}{q-1+(q+1)\sqrt{1-4qt^2}} \left(\frac{1-\sqrt{1-4t^2}}{2qt} \right)^r, \tag{27}$$

see [McK83] and [RZ09]; For $r \geq 0$, the exponential generating function

$$g_{q+1}(t) := e^{(q+1)t} H_{T_{q+1}}(x,y;t)$$

of the sequence $\{b_k(r)\}_{k=0}^{\infty}$ can be expressed in terms of the ordinary generating function in at least two different ways. In one approach, we start with the identity

$$t^{-1} f_{q+1}(t^{-1}) = (\mathcal{L} g_{q+1})(t),$$

which is valid for $|t| > 2\sqrt{q}$ and where $\mathcal{L}$ denotes the Laplace transform. With elementary algebraic manipulations, one obtains the identity that

$$(\mathcal{L} g_{q+1})(t) = \sum_{j=0}^{\infty} q^{-(r+2j)/2} \left(\frac{t-\sqrt{t^2-4q}}{2\sqrt{q}} \right)^{2j+r} \left(\frac{t-\sqrt{t^2-4q}}{2q} \right),$$

which is valid for $|t| > 2\sqrt{q}$. The identity

$$\left(\frac{t-\sqrt{t^2-4q}}{2q} \right) = \frac{1}{\sqrt{t^2-4q}} \left(1 - \left(\frac{t-\sqrt{t^2-4q}}{2\sqrt{q}} \right)^2 \right)$$

yields that

$$(\mathcal{L} g_{q+1})(t) = \frac{1}{\sqrt{t^2-4q}} \sum_{j=0}^{\infty} q^{-(r+2j)/2} \left(\frac{t-\sqrt{t^2-4q}}{2\sqrt{q}} \right)^{2j+r} \left(1 - q^{-1} \left(\frac{t-\sqrt{t^2-4q}}{2\sqrt{q}} \right)^2 \right),$$

which is valid for $|t| > 2\sqrt{q}$. Therefore,

$$(\mathcal{L} g_{q+1})(t) = \frac{q^{-r/2}}{\sqrt{t^2-4q}} \left(\frac{t-\sqrt{t^2-4q}}{2\sqrt{q}} \right)^r - (q-1) \sum_{j=1}^{\infty} \frac{q^{-(r+2j)/2}}{\sqrt{t^2-4q}} \left(\frac{t-\sqrt{t^2-4q}}{2\sqrt{q}} \right)^{2j+r}.$$

From [GR07], section 17.13, formula 109 with $a = 2\sqrt{q}$ and $\nu = r + 2j$ for $j = 0, 1, \ldots$ and $\mathrm{Re}(t) > 2\sqrt{q}$, we have that

$$\mathcal{L}(I_{r+2j}(2\sqrt{q}x))(t) = \frac{1}{\sqrt{t^2-4q}} \left(\frac{t-\sqrt{t^2-4q}}{2\sqrt{q}} \right)^{2j+r}.$$

From this, we conclude that

$$e^{(q+1)t} H_{T_{q+1}}(x, y; t) = q^{-r/2} I_r(2\sqrt{q}t) - (q-1) \sum_{j=1}^{\infty} q^{-(r+2j)/2} I_{2j+r}(2\sqrt{q}t). \tag{28}$$

The formula in (28) is precisely the expression for the heat kernel on a T_{q+1} which was first proved in [CJK15, Proposition 3.1].

As stated, the exponential generating function $g_{q+1}(t)$ and the ordinary generating function $f_{q+1}(t)$ are related by the Laplace transform, meaning that

$$g_{q+1}(t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f_{q+1}(te^{i\theta}) \exp(e^{i\theta}) d\theta,$$

valid for $|t| < 1/(2\sqrt{q})$. Using (27), one can employ elementary manipulations of the integral and derive the integral expression for the heat kernel $H_{T_{q+1}}(x, y; t)$ established in [CY99]. We will omit the details of these computations.

6 Using a distance metric to construct a parametrix

In this section we will describe how to define further examples of a parametrix for the heat kernel using a distance function on G. The examples we develop come from different distance functions $d : VG \times VG \to \mathbb{R}_{\geq 0}$, so we denote the parametrix by H_d. In section 6.1 we define some metrics that can be used in the construction of H_d, and in section 6.2 we give explicit examples of an associated parametrix.

Throughout this section, we assume that an infinite graph G satisfies assumptions (G1), (G2') and the following strengthening of the assumption (G3):

(G3') **Uniform boundedness of the combinatorial vertex degree.** There exists a positive integer N such that for all $x \in VG$ the number of $y \in VG$ such that $w_{xy} > 0$ is bounded by N.

Assumption (G3') is not unusual in the work that is related to properties of operators on infinite weighted graphs. For example, it suffices to deduce natural upper and lower bounds for the heat kernel in terms of the combinatorial distance in [MS00] and [Sc02]. Moreover, uniform boundedness of the combinatorial degree yields essential self-adjointness of the Laplacian, as well as of other operators on G, such as a Schrödinger operator. For more details, we refer to [CdVT-HT11] or [Mi11].

6.1 Distance metric on a weighted graph

Let $d_G(x, y)$ denote an arbitrary distance metric on G which is uniformly bounded from below. More specifically, we assume there is a positive constant δ such that

$$\text{for all } x, y \in VG \quad \text{we have that} \quad d_G(x, y) \geq \delta > 0. \tag{29}$$

Such a metric always exists on a connected graph, and below in this section, as well as in section 7.1, we will provide a few examples.

6.1.1 Combinatorial graph distance

The graph G is connected, meaning for any two distinct points $x, y \in VG$ there exists a path connecting the x to y. To be clear, by a path we mean a sequence of points $p(x, y) = \{x = x_0, x_1, \ldots, x_n = y\}$ such that $w_{x_j x_{j+1}} > 0$ for all $j \geq 0$. The path $p(x, y) = \{x = x_0, x_1, \ldots, x_n = y\}$ is of length $n \in \mathbb{N}$. If $d_G(x, y)$ denotes the minimal length of all paths that connect x and y, it is then straightforward to conclude that d_G is a distance metric on G. Indeed, d_G is well defined because G is connected. The function d_G is symmetric, which follows from the fact that G is undirected. Also, the triangle inequality is immediate, while the equivalence $d_G(x, y) = 0$ if and only if $x = y$ follows from the fact that G has no loops.

This distance metric will be called the *combinatorial graph distance*. It is obviously satisfies (29) with $\delta = 1$.

The combinatorial graph distance is *intrinsic* metric on G (as defined in [FLW14]) if and only if the condition (G3') is fulfilled, see [HKMW13] and [KLSW15].

6.1.2 Metric adapted to the Laplacian

There are another choices for a metric on G which in addition to satisfying (29) is closely related to stochastic properties of a graph. For example, *the normalized combinatorial graph distance* metric is defined by

$$\rho_G := (A(G, w, \theta))^{-1/2} d_G;$$

see (8) and section 6.1.1. It is immediate that ρ_G is bounded from below by $\delta = (M/\eta)^{-1/2}$. The metric ρ_G is *adapted to the Laplacian* Δ_G, in view of the Definition (1.3) on p. 117 of [Fo13]. This means that for all $x \in VG$, the metric ρ_G satisfies the inequality

$$\frac{1}{\theta(x)} \sum_{y \sim x} \rho_G^2(x, y) w_{xy} \leq 1 \tag{30}$$

and there exists a constant c_{ρ_G} such that $\rho_G(x, y) \leq c_{\rho_G}$ whenever $x \sim y$. The inequality (30) is analogous to the geodesic distance ρ on a Riemannian manifold which satisfies $|\nabla \rho(x, \cdot)| \leq 1$. Any metric on G adapted to the Laplacian is intrinsic.

A further example of a metric on G which is adopted to the Laplacian Δ_G and uniformly bounded from below is defined as follows. For all $x, y \in VG$, let

$$\tilde{d}_G(x, y) := \inf \left\{ \sum_{e \in p(x,y)} \min\{1, u(e)\} : p(x, y) \, \text{is a path joining } \, x \, \text{and} \, y \right\}$$

where e is an edge in the path and, if x_i and x_{i+1} are the endpoints of the edge e, $u(e)$ is defined as

$$u(e) = \left(\min \left\{ \frac{\theta(x_i)}{\mu(x_i)}, \frac{\theta(x_{i+1})}{\mu(x_{i+1})} \right\} \right)^{1/2}.$$

6.2 Dilated Gaussian as a parametrix

Let $d : VG \times VG \to [0, \infty)$ denote any distance metric on G satisfying the assumption (29).

Proposition 12. *With the notation as above, let* $H_d : VG \times VG \times (0, \infty) \to [0, \infty)$ *be defined as*

$$H_d(x, y; t) := \frac{1}{\sqrt{\theta(x)\theta(y)}} \exp(-(\theta(x)\theta(y) d^2(x, y))/t) \tag{31}$$

and

$$H_d(x,y;0) = \lim_{t\downarrow 0} H_d(x,y;t).$$

Then H_d is a parametrix for the heat operator on G of order $k=0$.

Proof. By assumption, the distance d is bounded from below. From this it is immediate that $H_d(x,y;t)$ is continuous function in t and that $H_d(x,y;0)=0$ satisfies (18). Trivially, $H_d(x,y;t)$ is smooth for $t\in(0,\infty)$ and all $x,y\in VG$. By definition, H_d is symmetric in the two spatial variables. So, in order to prove integrability in each space variable, it suffices to show that for all $y\in VG$ and $t>0$, we have that

$$\sum_{x\in VG} \exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t}\right)\sqrt{\frac{\theta(x)}{\theta(y)}} \leq \frac{1}{\sqrt{\eta}}\sum_{x\in VG}\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t}\right)\sqrt{\theta(x)} < \infty. \tag{32}$$

First, we note that for all positive numbers a and u, the inequality

$$u\exp(-u^2a^2) \leq \frac{1}{a\sqrt{2e}}$$

follows from elementary calculus. When taking $u=\sqrt{\theta(x)\theta(y)}d(x,y)$ for $x\neq y$ and $a=\frac{1}{\sqrt{2t}}$, we get that

$$\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{2t}\right)\sqrt{\theta(x)} \leq \sqrt{\frac{t}{e}}\frac{1}{\sqrt{\theta(y)}d(x,y)} \leq \frac{1}{\delta}\sqrt{\frac{t}{\eta e}},$$

where we used (G2') and (29) to deduce the last inequality. Therefore,

$$\sum_{x\in VG}\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t}\right)\sqrt{\theta(x)} \leq \sqrt{\theta(y)} + \sqrt{\frac{t}{\eta e}}\frac{1}{\delta}\sum_{x\in VG\setminus\{y\}}\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{2t}\right).$$

It is left to prove that the series on the right-hand side of the above equation converges. For this, note that when combining (G3') with (29) we conclude that for fixed y on G there are at most N^{n+1} vertices $x\neq y$ with distance $\leq (n+1)\delta$ from y. Therefore,

$$\begin{aligned}\sum_{x\in VG\setminus\{y\}}\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{2t}\right) &= \sum_{n=1}^{\infty}\sum_{n\delta<d(x,y)\leq(n+1)\delta}\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{2t}\right)\\ &\leq \sum_{n=1}^{\infty}N^{n+1}\exp\left(-\frac{(\eta n\delta)^2}{2t}\right)<\infty.\end{aligned} \tag{33}$$

This completes the proof that H_d is integrable in both space variables.

Next, we want to show the second condition in Definition 6 of the parametrix holds for H_d. By definition, for $t>0$ we have that

$$\begin{aligned}L_{G,x}H_d(x,y;t) = \frac{1}{\theta(x)}\sum_{z\sim x}&\left(\frac{1}{\sqrt{\theta(x)\theta(y)}}\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t}\right)\right.\\ &\left.-\frac{1}{\sqrt{\theta(z)\theta(y)}}\exp\left(-\frac{\theta(z)\theta(y)d^2(z,y)}{t}\right)\right)w_{xz}\\ &+\frac{\theta(x)\theta(y)d^2(x,y)}{t^2\sqrt{\theta(x)\theta(y)}}\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t}\right).\end{aligned} \tag{34}$$

The sum on the right-hand side (34) is finite by (G3'), and each term extends to a continuous function in $t \in [0, \infty)$. Therefore, the second condition in Definition 6 is also fulfilled.

Going further, conditions (G1) and (G2') yield that

$$\begin{aligned}|\Delta_{G,x} H_d(x,y;t)| &\leq \frac{M}{\eta^2} \sum_{z \sim x} \left(\exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t} \right) + \exp\left(-\frac{\theta(z)\theta(y)d^2(z,y)}{t} \right) \right) \\ &\leq \frac{2MN}{\eta^2}.\end{aligned}$$

For all $u, a > 0$, we have that

$$u^2 a^{-2} \exp(-u^2/a) \leq \frac{1}{ae},$$

and for $u > 0$,

$$\lim_{a \downarrow 0} u^2 a^{-2} \exp(-u^2/a) = 0.$$

Upon taking $u = \sqrt{\theta(x)\theta(y)} d(x,y)$ and $a = t$, we get for $x \neq y$ and $t \in (0, t_0)$ that

$$\begin{aligned}&\frac{\theta(x)\theta(y)d^2(x,y)}{t^2\sqrt{\theta(x)\theta(y)}} \exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t} \right) \\ &\qquad \leq \frac{1}{\eta} \frac{\theta(x)\theta(y)d^2(x,y)}{t^2} \exp\left(-\frac{(\sqrt{\theta(x)\theta(y)}d(x,y))^2}{t} \right) \leq \frac{C}{\eta},\end{aligned}$$

where C is a constant depending only on t_0. When $x = y$, the third line in (34) equals zero. With all this, we have proved that $L_{G,x} H_d(x,y;t)$ is bounded for $t \in (0, t_0)$ by a constant depending only on t_0.

Finally, in order to prove that H_d is the parametrix of order zero, it is left to prove that $\Delta_{G,x} H_d(x,\cdot;t)$ and $\frac{\partial}{\partial t} H_d(x,\cdot;t)$ are in $L^1(\theta)$ for $x \in VG$, $t > 0$. From (G1), (G2') and (G3') we get that

$$\begin{aligned}\sum_{y \in VG} |\Delta_{G,x} H_d(x,y;t)| \theta(y) &\leq \frac{MN}{\eta^{3/2}} \sum_{y \in VG} \exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t} \right) \sqrt{\theta(y)} \\ &\quad + \frac{M}{\eta^{3/2}} \sum_{z \sim x} \sum_{y \in VG} \exp\left(-\frac{\theta(z)\theta(y)d^2(z,y)^2}{t} \right) \sqrt{\theta(y)}.\end{aligned} \tag{35}$$

In view of (G3') and the symmetry of variables, it follows from (32) that all series on the right-hand side (35) are finite. This proves that $\Delta_{G,x} H_d(x,\cdot;t) \in L^1(\theta)$.

To complete the proof of the proposition it is left to show that

$$\sum_{y \in VG} \frac{\theta(x)\theta(y)d^2(x,y)}{t^2\sqrt{\theta(x)\theta(y)}} \exp\left(-\frac{\theta(x)\theta(y)d^2(x,y)}{t} \right) \theta(y) < \infty.$$

The proof is completely analogous to the proof of (32), so we will omit further details.

□

Remark 13. In Proposition 12 above, the choice of a distance metric was not specified. Indeed, any distance metric d which is uniformly bounded from below could be used in the definition (31) for the parametrix. In other words, we can construct the same heat kernel when using different distance metric on the graph.

This is quite different from the Riemannian manifolds situation where the construction of a parametrix already requires considerable local information associated to the Laplacian; see, for example, section VI.4 of [Ch84]. In a sense, the very general methods by which one can define a parametrix for an infinite graph belongs to a class of geometric phenomena on the graph which are somewhat unexpected if one were to view a graph as the discretization of a manifold. For an extensive discussion of such phenomena we refer to [KLW21].

7 Concluding remarks

We will close this article with the following observations.

7.1 Edge-weighted graph distance

In order to satisfy condition (29), one could impose the following condition.

(E1) **Boundedness from below of the edge weight:** There exists a positive integer $\tilde{\delta}$ such that

$$\inf_{x,y\in VG;x\neq y} w_{xy} > \tilde{\delta}.$$

Condition (E1) when combined with (G1) yields (G3'). As such, the parametrix construction for the heat kernel described in the preceding section can be carried out with a distance metric which satisfies conditions (G1), (G2') and (E1).

Assumption (E1) arises naturally in the context of metric graphs in which a positive real number ℓ_e is associated to every edge $e = \{x, y\}$ of a graph, so then w_{xy} can be taken be equal ℓ_e. The condition $\inf_e \ell_e > 0$ is then imposed in order to deduce that a connected metric graph is actually a length metric space; see for example [BBI01] or [St06].

With (E1) another distance on G can be defined as follows. For any vertices x and y and any path $p(x, y) = \{x = x_0, x_1, \ldots, x_n = y\}$ connecting points x and y, the *weighted length* of the path $\ell_w(p(x, y))$ is defined by

$$\ell_w(p(x,y)) := \sum_{j\geq 0} w_{x_j x_{j+1}}.$$

Let

$$\tilde{d}_G(x,y) := \inf_{p(x,y)} \ell_w(p(x,y))$$

where the infimum is taken over all paths connecting x and y. Since G is connected and w_{xy} is uniformly bounded from below, the function $\tilde{d}_G : VG \times VG \to [0, \infty]$ is a distance on VG which can be called the *edge-weighted distance*. For graphs satisfying (G1), (G2') and (E1) it is immediate that the dilated Gaussian $H_{\tilde{d}_G}$ defined by (31) is a parametrix.

7.2 Construction of the resolvent kernel

The resolvent kernel, or the Green's function, associated to the graph Laplacian can be expressed as the Laplace transform of the heat kernel (possibly truncated by the contribution from the eigenvalue zero), see e.g. [CY00]. Applying the formula 3.478.4 of [GR07] with $\nu = p = 1$, the expression for the heat kernel with the "seed" H_d can be used in order to deduce an explicit expression for the resolvent kernel in terms of series of products of K-Bessel functions with index 1. We will exploit this construction of the resolvent kernel in a subsequent article.

In case one is interested in computing the resolvent kernel of a subgraph G' of an infinite graph G, one may start with the heat kernel H_G on G as a parametrix and use it to derive the heat kernel on G' as described in Theorem 8 above. Then, by taking the Laplace transform of this expression (possibly truncated by the contribution from the eigenvalue zero) one will be able to express the resolvent kernel on G' in terms of the resolvent kernel on G, see e.g. [LNY22] for the case of a subgraph of a complete graph.

7.3 Varying edge and vertex weights

For a given graph G, with the edge weights function w let $H_{G,w}$ be the heat kernel associated to the edge weights function w. Let w' denote another edge weights function on G, and $H_{G,w'}$ be the associated heat kernel. Then $H_{G,w}$ can be used as a parametrix for the heat kernel on (G, w'). In fact, the convolution series in Theorem 8 gives a precise formula for the difference

$$H_{G,w'}(x, y; t) - H_{G,w}(x, y; t).$$

From this expression, it is possible to study the variation of the heat kernel in w, from which one could study spectral invariants derived from the heat kernel such as regularized determinants or asymptotic behavior as, say, one edge weight approaches zero.

For a given graph G, with the vertex weights functions θ, θ' let $H_{G,\theta}$, $H_{G,\theta'}$ be the corresponding heat kernels. Then, $\sqrt{\frac{\theta(x)\theta(y)}{\theta'(x)\theta'(y)}}H_{G,\theta}(x, y; t)$ can be used as a parametrix for the heat kernel on (G, θ').

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