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THE SPREAD OF THE POTENTIAL ON A WEIGHTED GRAPH

Abstract.
We compute explicitly the solution of the heat equation on a weighted graph Γ whose edges are identified with copies of the segment [0, 1] with the condition that the sum of the weighted normal exterior derivatives is 0 at every node (Kirchhoff type condition).

1. Introduction

In our previous papers [1], [2] we studied the diffusion equation

$$\frac{\partial V}{\partial t} = \frac{\partial^2 V}{\partial x^2} - V \tag{1}$$

on a continuous structure defined on a weighted graph $\Gamma = (V, E)$ whose vertices satisfy Kirchhoff type conditions. This model arises in neurobiology. It models the spread of the potential along the ramifications of a neuron.

In [2] we determined the heat kernel on the above mentioned continuous structure when Γ is a homogeneous tree. The purpose of this note is to extend the results of [2] to the case of a generic countable graph whose vertices have uniformly bounded degrees (for finite graph see J.P. Roth, ref. [8]). This wider generality is achieved essentially by the same techniques developed in the case of the homogeneous tree. Its main interest lies in the fact that we are able to describe the heat kernel for all the general structures we studied in [1]. In that paper we determined the spectrum of the continuous Laplacian Δ with only mild assumptions on Γ and its weights. The present note, because of its greater generality, is thus a better companion to [1] than the previous paper [2] was. Moreover, at the best of our knowledge, it seems to represent the state of the art of the subject at this level of generality.

We remark that our entire approach to the subject (in [1], [2] and in the present note) is in the line of previous work by J.P. Roth (see [8]). A different but related kind of analysis can be found in papers by B. Gaveau, M. Okada and T. Okada (see [3], [6]). They study the heat kernel on several examples of $1-$dimensional structures. Some of these structures, namely homogeneous trees (and skew homogeneous trees in [6] example 4) and networks ([3] models X_{10} and X_{12}), after maybe some renormalization, are particular cases of our weighted graphs. So, for example, in [6], T. Okada considers homogeneous trees of degree 3 with weights distributed in a periodic (but not symmetric) fashion. For that example, nice asymptotic estimares are proved and the generalization to homogeneous trees of any degrees with "periodic weights" is easily within reach by the same techniques.

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Our estimates are much cruder, but they apply to all graphs with randomly distributed weights. Even for homogeneous trees, Okada's techniques do not seem to work once we deal with general (non periodic, non symmetric) weight distributions. To improve our estimates on the general setting further work and new ideas seem necessary.

In order to keep this note (we stress again that it should be thought as an improved and completed version of [2]) relatively selfcontained, in section 2 we introduce notation and basic facts. Namely, we describe the graph Γ as a CW-complex, so that we can introduce a natural topology on Γ. We assign conductances to the edges of Γ and require them to satisfy a suitable uniformity condition. We set Kirchhoff type conditions at the vertices of Γ, we define the spaces $L^2(\Gamma, c)$ and $H^m(\Gamma, c)$ and describe the domain of the continuous Laplacian Δ and its basic properties. Finally we prove Lemma 1. It was by realizing that the estimate in Lemma 1 of [2] actually holds in the general setting of the present note (uniformly bounded degrees) that the whole generalization became possible. We remark, however that Lemma 1 is far from being optimal. We believe that substantial improvement of that Lemma would allow a deeper analysis of the subject especially with regard to the behavior as $t \to \infty$.

Section 3, where we determine the heat kernel on Γ and the solution of the Cauchy problem associated to the diffusion equation (1), is mainly a list of results and it strictly parallels [2]. We omit the proofs since they are similar to the corresponding ones in [2] with the new version of Lemma 1 replacing its analogous in [2].

2. Notation and Preliminaries

Let $\Gamma = (V, E)$ be a countable, connected graph with no self-loops and uniformly bounded degrees (i.e. there exists a constant d such that $1 \le d_v \le d < \infty$ for every vertex v in V, where d_v is the degree of v).

We say that two edges e and e' are neighbours and we write $e \sim e'$ if they have a common endpoint (i.e. a common vertex).

We identify every edge e of Γ with the real interval [0, 1]. In this way we associate with Γ an one-dimensional CW-complex (see e.g. J.R. Munkres, ref. [5]). Note that Γ is a metric space in a natural way.

We can orient every edge e of Γ in two opposite ways. For every edge e, we denote by $+e$ and $-e$ the two opposite orientations and by $\mid e \mid$ the edge e (unoriented). If no confusion can arise, we denote by e both the oriented and the unoriented edge e. For every oriented edge (arc) e we denote by $I(e)$ the initial vertex of e, by $T(e)$ the terminal vertex.

We define a path C to be a finite sequence of arcs $(e_1, \ldots, e_m)$ $(m > 1)$ such that $T(e_j) = I(e_{j+1})$ for $1 \le j \le m-1$. We call length of the path C, denoted by $l(C)$, the number of the arcs of C. We denote by $\mathbf{C}$ the set of all the paths on Γ.

Let e and e' be two edges of Γ. We denote by $\mathbf{C}_m(e, e')$ the set of all the paths having length m whose first arc is one of two arcs obtained by e and whose last arc is one of two arcs obtained by e' i.e.

$$\mathbf{C}_m(e, e') = \{C \in \mathbf{C} : l(C) = m \quad \text{and} \quad C = (\pm e, e_1, \ldots, e_{m-2}, \pm e')\} \tag{2}$$

LEMMA 1. *For all m*

$$\operatorname{card}(\boldsymbol{C}_m(e, e')) \le 2d^{m-1}$$

where $d = \sup_{v \in V} d_v$

Proof. Let $\mathbf{C}_m(e)$ be the set of all the paths having length m and whose first arc is one of two arcs obtained by the edge e i.e.

$$\mathbf{C}_m(e) = \{C \in \mathbf{C} : l(C) = m \quad \text{and} \quad C = (\pm e, e_1, \ldots, e_{m-1})\}$$

The paths of $\mathbf{C}_m(e, e')$ are particular paths of $\mathbf{C}_m(e)$, so it is enough to evaluate the cardinality of $\mathbf{C}_m(e)$. We observe that $\mathbf{C}_1(e)$ has exactly 2 elements. Every path of $C_{m+1}(e)$ comes from a path of $C_m(e)$. Moreover if we fix a path $(\pm e, e_1, \ldots, e_{m-1})$ of $\mathbf{C}_m(e)$, then there exist at most d paths of $C_{m+1}(e)$ coming from it (each of these paths is obtained by adding to $(\pm e, e_1, \ldots, e_{m-1})$ any one of the arcs branching out from $T(e_{m-1})$). So

$$\operatorname{card}(\mathbf{C}_m(e, e')) \leq \operatorname{card}(\mathbf{C}_m(e)) \leq 2d^{m-1}$$

□

If x and y are points of the same edge, let us denote by $\mid x - y \mid$ the (euclidean) distance between x and y.

For every point x of Γ, we denote by E_x the set of all the edges containing x.

Let x and y be points of Γ. We call geodesic path joining x to y any path of minimum length whose first and last arcs are obteined from edges of E_x and E_y respectively. Geodesic paths from x to y may not be unique, but we denote by $l^\star$ their common length.

Set

(3) $$\rho(x, y) = \begin{cases} 0 & \text{if } x \text{ and } y \text{ belong to the same edge} \\ l^* - 2 & \text{otherwise} \end{cases}$$

or

$$\rho(x, y) = \max\{0, (l^\star - 2)\}$$

We assign to every edge e of Γ a positive conductance $c(e)$ in such a way that

(4) $$\frac{c(e)}{c(e')} \leq \kappa \quad \text{if the edges } e, e' \text{ are neighbours}$$

where $\kappa \geq 1$.

For every vertex v of Γ we denote by $c(v)$ the sum of the conductances of all the edges branching out from v i.e.

$$c(v) = \sum_{e \in E_v} c(e)$$

We call the following quantity transfer coefficient from the arc e to the arc e'

(5) $$\varepsilon_{e,e'} = \begin{cases} 2c(\mid e \mid)/c(T(e)) & \text{if} T(e) = I(e'), e' \neq -e \\ 2c(\mid e \mid)/c(T(e)) - 1 & \text{if} T(e) = I(e'), e' = -e \\ 0 & \text{if} T(e) \neq I(e') \end{cases}$$

We observe that

$$|\varepsilon_{e,e'}| \leq \kappa$$

and

$$c(\mid e \mid)^{-1} \varepsilon_{e,e'} = c(\mid e' \mid=)^{-1} \varepsilon_{-e',-e}$$

As consequence of this equality the heat kernel turns out to be symmetric with respect to the space variables.

For every path $C = (e_1, \dots, e_m)$ $(m > 1)$ on Γ, we denote by ε_C the product of the transfer coefficients of all the pairs of consecutive arcs of C i.e.

$$\varepsilon_C = \prod_{j=1}^{m-1} \varepsilon_{e_j, e_{j+1}} \tag{6}$$

We denote by $\mathbb{R}_+$ the set of the real numbers which are strictly positive.

Let $k(t, x)$ be the source solution of the heat equation on $\mathbb{R}$

$$k(t,x) = \begin{cases} \frac{1}{2\sqrt{\pi t}} \exp(-x^2/4t) & \text{if}(t,x) \in \mathbb{R}_+ \times \mathbb{R} \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

and set

$$h(t,x) = \frac{x}{t} k(t,x) \tag{8}$$

We will identify any function u on Γ with a collection $\{u_e\}_{e \in E}$ of functions u_e defined on the edges e of Γ. Note that u_e can be considered a function on $[0, 1]$. In fact, we will use the same notation u_e to denote both the function on the edge e and the function on the real interval $[0, 1]$ identified with e.

The integral on Γ of a positive function u is defined as follows

$$\int_\Gamma u(x)dx = \sum_{e \in = E} c(e) \int_e u_e(x)dx = \sum_{e \in = E} c(e) \int_0^1 u_e(x)dx$$

We define the space $L^2(\Gamma, c)$ as the space of all the collections $u = \{u_e\}_{e \in E}$ on Γ such that $u_e \in L^2((0, 1))$ for every e in E, and $\sum_{e \in E} c(e) \parallel u_e \parallel^2_{L^2((0,1))} < \infty$.

Analogously, for every integer $m > 0$, we define the Sobolev space $H^m(\Gamma, c)$ as the space of all the collections $u = \{u_e\}_{e \in E}$ on Γ such that u is continuous on Γ, $u_e \in H^m((0, 1))$ for every e in E, and $\sum_{e \in E} c(e) \parallel u_e \parallel^2_{H^m((0,1))} < \infty$.

It is easy to see that the above spaces are Hilbert spaces.

Consider the sesquilinear continuous form φ on $H^1(\Gamma, c)$ defined by

$$\varphi(u, w) = (u', w')_{L^2(\Gamma, c)}$$

and let Δ be its associated Laplacian.

It is not difficult to prove that the operator Δ is defined on the set $D(\Delta)$ of all the collections $u = \{u_e\}_{e \in E}$ of $H^2(\Gamma, c)$ satisfying the Kirchhoff type conditions at every vertex v of V namely

$$D(\Delta) = \{u \in H^2(\Gamma, c) : \sum_{e \in E_v} c(e) \frac{\partial u_e}{\partial n_e}(v) = 0 \quad \text{for all } v \text{ in } V\}$$

where $\frac{\partial u_e}{\partial n_e}(v)$ denotes the normal exterior derivative of u_e evaluated at v i.e.

$$\frac{\partial u_e}{\partial n_e}(v) = \begin{cases} -\lim_{h \to 0^+} (u_e(h) - u_e(0))/h & \text{if v=0} \\ \lim_{h \to 0^-} (u_e(h+1) - u_e(1))/h & \text{if v=1} \end{cases}$$

Moreover for every function $u = \{u_e\}_{e \in E}$ in $D(\Delta)$ and for every edge e in E we have that

$$(\Delta u)_e = u''{}_e$$

3. The heat kernel and the solution of the Cauchy problem

Our aim is to determine the heat kernel and the solution of the Cauchy problem

$$\text{(9)} \qquad \begin{cases} \frac{\partial u}{\partial t} & = & \Delta u - u \quad t > 0 \\ u(0) & = & f \end{cases}$$

where f belongs to $L^2(\Gamma, c)$.

By the theory of semigroups (see e.g. A. Pazy, ref. [7]) we know that if $P_t f$ is the solution of the Cauchy problem

$$\text{(10)} \qquad \begin{cases} \frac{\partial u}{\partial t} & = & \Delta u \quad t > 0 \\ u(0) & = & f \end{cases}$$

then $(\exp(-t))P_t f$ is the solution of (9). Since $P_t f$ is the integral over Γ of f against the heat kernel, we first compute the heat kernel.

Let x and y be in Γ. Choose any e, e' in E such that $x \in e$ and $y \in e'$. With the notation of (2), (3), (6), (7) set

$$\text{(11)} \qquad K(t, x, y) = c(e)^{-1} k(t, \mid x - y \mid) \delta_{e,e'} + L(t, x, y)$$

where

$$\delta_{e,e'} = \begin{cases} 1 & \text{if} e' = e \\ 0 & \text{otherwise} \end{cases}$$

and

$$L(t, x, y) = c(e)^{-1} \sum_{m \geq \rho(x,y)} \sum_{C \in \mathbf{C}_{m+2}(e,e')} \varepsilon_C k(t, \mid x - T(\pm e) \mid + m + \mid y - I(\pm e') \mid)$$

Next theorem shows that K is the heat kernel on Γ.

THEOREM 1. *The function K defined in (11) does not depend on e and e' and has the following properties*

(i) $\frac{\partial K}{\partial y}(t, x, y)$ *and* $\frac{\partial^2 K}{\partial y^2}(t, x, y)$ *exist on* $\mathbb{R}_+ \times \Gamma \times (\Gamma \setminus V)$

(ii) $\frac{\partial K}{\partial t}(\cdot, x, y)$ *exists continuous on* $\mathbb{R}_+$ *for every* (x, y) *in* $\Gamma \times (\Gamma \setminus V)$

(iii) $\frac{\partial K}{\partial t}(t, x, y) = \frac{\partial^2 K}{\partial y^2}(t, x, y)$ *on* $\mathbb{R}_+ \times \Gamma \times (\Gamma \setminus V)$

(iv) $K(t, x, \cdot) \in D(\Delta)$ *for every* (t, x) *in* $\mathbb{R}_+ \times \Gamma$

REMARK 1. One can prove, essentially repeating the procedure adopted by J.P. Roth (see ref.[8]), that if there exists a function $H(t, x, y)$ with the properties of Theorem 1, then, for every (t, x, y) in $R_+ \times \Gamma \times \Gamma$ we have

$$H(t, x, y) = K(t, x, y)$$

Therefore we can consider the properties listed in Theorem 1 as the properties characterizing the fundamental solution of the heat equation on Γ.

The proof of Theorem 1 depends on the estimates in the following Lemmas.

LEMMA 2. *There exist $\eta > 0$ and $\nu > 0$ (independent of e and e') such that, for every (t, x, y) in $R_+ \times \Gamma \times \Gamma$*

$$(12) \qquad \begin{aligned} | L(t, x, y) | &\leq \frac{\kappa d}{c(e)\sqrt{\pi t}} \sum_{m \geq \rho(x,y)} \exp\left(m(\ln \kappa d) - m/4t\right) \\ &\leq \frac{\eta}{c(e)\sqrt{t}}(1+t)\exp(\nu t) \end{aligned}$$

(κ is as in (4))

Moreover there exist $t_0 > 0$ and $\alpha > 0$ (independent of e and e') such that, for all (t, x, y) in $(0, t_0] \times \Gamma \times \Gamma$

$$| L(t, x, y) | \leq \frac{\alpha}{c(e)\sqrt{t}} \exp\left(-\rho^2(x, y)\beta/t\right)$$

where $\frac{1}{8} < \beta < \frac{1}{4}$.

In order to compute $\frac{\partial K}{\partial y}(t, x, y)$ and $\frac{\partial^2 K}{\partial y^2}(t, x, y)$ we determine $\frac{\partial L}{\partial y}(t, x, y)$ and $\frac{\partial^2 L}{\partial y^2}(t, x, y)$ and study their regularity. With x, y, e and e' as above set

$$\begin{aligned} L_1(t, x, y) &= c(e)^{-1} \textstyle\sum_{m \geq \rho(x,y)} \sum_{C \in \mathbf{C}_{m+2}(e,e')} \\ &= \varepsilon_C \frac{\partial k}{\partial y}(t, | x - T(\pm e) | +m+ | y - I(\pm e') |) \end{aligned}$$

and

$$\begin{aligned} L_2(t, x, y) = {} & c(e)^{-1} \textstyle\sum_{m \geq \rho(x,y)} \sum_{C \in \mathbf{C}_{m+2}(e,e')} \\ & \varepsilon_C \frac{\partial^2 k}{\partial y^2}(t, | x - T(\pm e) | +m+ | y - I(\pm e') |) \end{aligned}$$

We have

LEMMA 3. *There exist $\eta > 0$ and $\nu > 0$ (independent of e and e') such that, for every (t, x, y) in $\mathbb{R}_+ \times \Gamma \times \Gamma$*

$$(i) \qquad \begin{aligned} | L_1(t, x, y) | &\leq \frac{e^2(\kappa d)}{2c(e)t\sqrt{\pi t}} \textstyle\sum_{m \geq \rho(x,y)} \exp\left(m(\ln(\kappa d) + 1 - m/4t)\right) \\ &\leq \frac{\eta}{c(e)t\sqrt{t}}(1+t)\exp(\nu t) \end{aligned}$$

For every (t, x) fixed in $R_+ \times \Gamma$ and for every y in e'

$$(ii) \qquad \frac{\partial L}{\partial y}(t, x, y) = L_1(t, x, y)$$

Moreover there exist $t_0 > 0$ *and* $\alpha > 0$ *(independent of e and e′) such that, for all* (t, x, y) *in* $(0, t_0] \times \Gamma \times \Gamma$

$$(iii) \qquad \left| \frac{\partial L}{\partial y}(t, x, y) \right| \leq \frac{\alpha}{c(e)t\sqrt{t}} \exp\left(-\rho^2(x, y)\beta/t\right)$$

where $\frac{1}{8} < \beta < \frac{1}{4}$.

and

LEMMA 4. *Set* $\tau = \min\{t, t^2\}$. *There exist* $\eta > 0$ *and* $\nu > 0$ *(independent of e and e′) such that, for every* (t, x, y) *in* $R_+ \times \Gamma \times \Gamma$

$$\begin{aligned} | L_2(t, x, y) | &\leq \frac{e^4(\kappa d)}{c(e)\tau\sqrt{\pi t}} \sum_{m \geq \rho(x,y)} \exp\left(m(\ln(\kappa d) + 2 - m/4t)\right) \\ &\leq \frac{\eta}{c(e)\tau\sqrt{t}}(1 + t)\exp(\nu t) \end{aligned}$$

For every (t, x) *fixed in* $R_+ \times \Gamma$ *and for every y in* e'

$$(ii) \qquad \frac{\partial^2 L}{\partial y^2}(t, x, y) = L_2(t, x, y)$$

Moreover there exist $t_0 > 0$ *and* $\alpha > 0$ *(independent of e and e′) such that, for all* (t, x, y) *in* $(0, t_0] \times \Gamma \times \Gamma$

$$(iii) \qquad \left| \frac{\partial^2 L}{\partial y^2}(t, x, y) \right| \leq \frac{\alpha}{c(e)t^2\sqrt{t}} \exp\left(-\rho^2(x, y)\beta/t\right)$$

where $\frac{1}{8} < \beta < \frac{1}{4}$.

We denote by $M(t, x)$ any one of the following functions $K(t, x, \cdot)$, $\frac{\partial K}{\partial y}(t, x, \cdot)$ and $\frac{\partial^2 K}{\partial y^2}(t, x, \cdot)$ then

LEMMA 5. *For the function* $M(t, x, y)$ *we have*

(i) $M(t, x, \cdot) \in L^1(\Gamma, c) \bigcap L^2(\Gamma, c)$ *for every*(t, x)*in*$\mathbb{R}_+ \times \Gamma$

(ii) there exists $\alpha_1(t) > 0$ *such that, for every x in* Γ

$$\| M(t, x, \cdot) \|_{L^1(\Gamma,c)} \leq \alpha_1(t)$$

(iii) there exists $\alpha_2(t) > 0$ *such that, for every x in* Γ

$$\| M(t, x, \cdot) \|_{L^2(\Gamma,c)} \leq \frac{\alpha_2(t)}{\min_{e \in E_x} c(e)}$$

REMARK 2. Lemma 5 still holds with the function $M(t, \cdot, y)$ replacing the function $M(t, x, \cdot)$ (where it is defined) and $c(e')$ instead of $c(e)$.

The proofs of the above results are essentially the same as the corresponding ones in [2]. We need only to modify the evaluation of the cardinality of the set $\mathbf{C}_m(e, e')$ and the absolute value of the transfer coefficient $\varepsilon_{e,e'}$. Therefore we omit them and refer to [2].

We conclude by solving the Cauchy problem (10) (again we refer to [2] for the proofs) For every f in $L^2(\Gamma, c)$ and for all y in Γ, set

$$P_t f(y) = \begin{cases} \int_\Gamma K(t,x,y) f(x)dx & if \quad t > 0 \\ f(y) & if \quad t = 0 \end{cases} \tag{13}$$

This definition makes sense since we have

PROPOSITION 1. *For every function f in $L^2(\Gamma, c)$ and for every $t > 0$ we have that the integral $\int_\Gamma M(t,x,y) f(x)dx$ exists for every y in $(\Gamma \setminus V)$ and*

$$\int_\Gamma M(t,x,\cdot) f(x)dx \in L^2(\Gamma, c)$$

(Recall that $M(t,x,y)$ denotes any one of three functions $K(t,x,y)$, $\frac{\partial K}{\partial y}(t,x,y)$, $\frac{\partial^2 K}{\partial y^2}(t,x,y)$).

Finally we can state

THEOREM 2. *$P_t f$ is the solution of the abstract Cauchy problem* (8)*, i.e. $P_t f$ has the following properties*

(i) $$P_t f(\cdot) \in D(\Delta) \quad for \quad t > 0$$

(ii) $$P_t f \quad \text{satisfies system} \quad (8)$$

(iii) $$P_t f \quad \text{is a continuous } L^2(\Gamma, c) \text{ valued function on} \quad (R_+ \bigcup \{0\})$$

(iv) $$P_t f \quad \text{is a continuously differentiable } L^2(\Gamma, c) \text{ valued function on} \quad R_+$$

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