The heat kernel on metric graphs and its geometric significance

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Analysis and Mathematical Physics 2024

Metric graphs

Introducing metric graphs – #1

Figure: Valentina Vetturi, *Tails*, 2023

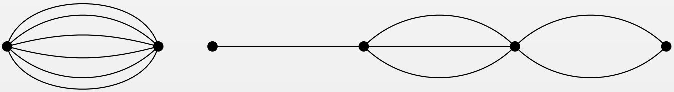
Introducing metric graphs – #2

Let

- $\mathsf{E} = \{\mathsf{e}_1, \mathsf{e}_2, \dots\}$ finite or countably infinite set ("edge set")
- $\ell : \mathsf{E} \to (0, \infty)$ ("edge lengths")
- $\sim$ equivalence relation on $\mathcal{V} := \bigsqcup_{\mathsf{e}\in\mathsf{E}} \{0, \ell_\mathsf{e}\}$ ("wiring")

  Define $\mathcal{E} := \bigsqcup_{\mathsf{e}\in\mathsf{E}} [0, \ell_\mathsf{e}]$ and extend canonically $\sim$ to $\mathcal{E}$.

  Then $\mathcal{G} := {}^{\mathcal{E}}\!/_{\sim}$ is a **metric graph**.



Its **vertex set** is $\mathsf{V} := {}^{\mathcal{V}}\!/_{\sim}$; its **volume** is $|\mathcal{G}| := \sum_{\mathsf{e}\in\mathsf{E}} \ell_\mathsf{e}$.

$\mathcal{G}$ as a metric measure space

Introduce the function spaces $C(\mathcal{G})$ and $L^p(\mathcal{G})$, $1 \le p \le \infty$, as well as

$$H^1(\mathcal{G}) := \{f \in C(\mathcal{G}) \cap L^2(\mathcal{G}) : f' \in L^2(\mathcal{G})\}.$$

The *bounded geometry* case: $0 < \inf_{e \in \ell_e}$ and $\sup_{e \in \ell_e} < \infty$

Lemma (Nicaise 1987?; Berkolaiko–Kuchment 2013?)

$$\mathfrak{a}(f) := \int_{\mathcal{G}} |f'|^2 \,\mathrm{d}x, \qquad f \in \mathrm{dom}(\mathfrak{a}) := H^1(\mathcal{G})$$

is a closed quadratic form.

The Laplacian $\Delta^{\mathcal{G}}$ is the self-adjoint operator on $L^2(\mathcal{G})$ associated with $\mathfrak{a}$.

Proposition (Kramar–M.–Sikolya 2007)

$\left(\mathfrak{a}, H^1(\mathcal{G})\right)$ *is a Dirichlet form; irreducible if* $\mathcal{G}$ *is connected.*

Recall: the heat kernel $p(t, \cdot, y)$ associated with a Laplacian Δ is the unique solution of

$$\begin{cases} \dfrac{\partial u}{\partial t}(t, \cdot) = \Delta u(t, \cdot), \\ u(0, \cdot) = \delta_y(\cdot) \end{cases}$$

By Mercer's Theorem, heat kernels are associated with Laplacians

- with Dirichlet BCs, on open $\Omega \subset \mathbb{R}^d$;
- with Neumann BCs, on open Lipschitz $\Omega \subset \mathbb{R}^d$;
- on smooth compact manifolds without boundary;
- ...

Lemma (Roth 1984; Cattaneo 1999)

$\Delta^{\mathcal{G}}$ is associated with a heat kernel $p^{\mathcal{G}}$, i.e.,

$$\mathrm{e}^{t\Delta^{\mathcal{G}}} f(x) = \int_{\mathcal{G}} p_t^{\mathcal{G}}(x,y) f(y)\,\mathrm{d}y, \qquad t > 0.$$

Moreover, $p^{\mathcal{G}} \in L^\infty(\mathcal{G} \times \mathcal{G})$.

Proof.

$H^1(\mathcal{G}) \hookrightarrow L^\infty(\mathcal{G})$ + Kantorovitch–Vulikh Theorem □

Definition (Directed paths)

(i) Either orientation $\vec{e}$ of an edge e is a *bond*

(ii) $\partial^-(\vec{e})$ (resp. $\partial^+(\vec{e})$) denotes the *initial* (resp. the *final*) vertex of $\vec{e}$; $\vec{e}_1, \vec{e}_2$ are *consecutive* if $\partial^+(\vec{e}_1) = \partial^-(\vec{e}_2)$.

(iii) Let $v, w \in V$. A *directed path* $\vec{p}$ is an sequence of consecutive bonds

$$\vec{p} = \big(v, \vec{e}_1, \ldots, \vec{e}_n, w\big)$$

such that $\partial^-(\vec{e}_1) = v$ and $\partial^+(\vec{e}_n) = w$.

Notation: $\mathcal{P}(v, w)$ is the set of *all directed paths* between v and w.

Theorem (Roth 1984; Borthwick–Harrell–Jones 2023)

If E *is finite, the heat kernel of* $\Delta^{\mathcal{G}}$ *is given by*

$$p_t^{\mathcal{G}}(x,y) = \frac{1}{\sqrt{4\pi t}} \sum_{\vec{p}\in\mathcal{P}(x,y)} \alpha(\vec{p}) \mathrm{e}^{-\frac{\mathrm{length}(\vec{p})^2}{4t}}, \qquad \forall t>0,\ x,y\in\mathcal{G}.$$

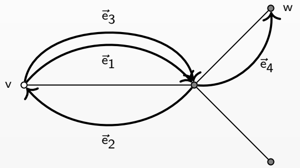
Here

$$\alpha(\vec{p}) := \prod_{k=1}^{n-1} \beta(\vec{\mathsf{e}}_k, \vec{\mathsf{e}}_{k+1}),$$

where

$$\beta(\vec{\mathsf{e}}_k, \vec{\mathsf{e}}_{k+1}) := \begin{cases} \frac{2}{\deg_{\mathcal{G}}(\partial^+(\vec{\mathsf{e}}_k))} - \delta_{\mathsf{e}_k,\mathsf{e}_{k+1}}, & \text{if } \partial^+(\mathsf{e}_k) \in \mathsf{V}\setminus \mathsf{V}^{\mathrm{D}}, \\ -1, & \text{if } \partial^+(\mathsf{e}_k)\in \mathsf{V}^{\mathrm{D}}. \end{cases}$$

Example



For $\vec{p} = (\mathsf{v}, \vec{e}_1, \vec{e}_2, \vec{e}_3, \vec{e}_4, \mathsf{w}) \in \mathcal{P}(\mathsf{v}, \mathsf{w})$ *one has*

$$\alpha(\vec{p}) = \beta(\vec{e}_1, \vec{e}_2) \cdot \beta(\vec{e}_2, \vec{e}_3) \cdot \beta(\vec{e}_3, \vec{e}_4)$$
$$= \left(\frac{2}{3} - 1\right) \cdot (-1) \cdot \frac{2}{3} = \frac{2}{9}.$$

More generally, $\alpha(\vec{p}) \in [-1, 1]$.

Corollary (Cattaneo 1999; Becker–Gregorio–M. 2021)

Roth's formula extends to infinite graphs of bounded geometry.

In the bounded geometry case, $\mathcal{G}$ is a geodesic space: for any $x, y \in \mathcal{G}$ there is a path $\vec{p}_{x,y}$ of minimal length.

Proposition (M. 2007; Haeseler 2013)

$$0 < p_t^{\mathcal{G}}(x,y) \leq \frac{c}{\sqrt{t}} \mathrm{e}^{-b\frac{\mathrm{length}(\vec{p}_{x,y})^2}{4t}} \qquad \forall t \in (0,1],\ x,y \in \mathcal{G}.$$

(Proof based on Davies' trick. Is there a proof based on Roth's formula?)

Two functionals on $\Omega \subset \mathbb{R}^d$ (Dirichlet)

$$\int_{\mathcal{G}} \langle \mathrm{e}^{t\Delta}\delta_x, \delta_x \rangle \,\mathrm{d}x = \int_{\mathcal{G}} p_t(x,x)\,\mathrm{d}x =: \mathrm{HeatTrace}(t,\Delta)$$

$$\|\mathrm{e}^{t\Delta}\mathbb{1}\|_{L^1} = \int_{\mathcal{G}}\int_{\mathcal{G}} p_t(x,y)\,\mathrm{d}x\,\mathrm{d}y =: \mathrm{HeatContent}(t,\Delta)$$

By the semigroup property + Gaussian estimates of $\mathrm{e}^{t\Delta}$ on $\Omega \subset \mathbb{R}^d$

$$ct^{\frac{d}{2}}\mathrm{HeatTrace}(t,\Delta) \leq \mathrm{HeatContent}(t,\Delta) \leq |\Omega|$$

Does it also hold $\mathrm{HeatTrace}(t,\Delta) < \infty \Rightarrow \mathrm{HeatContent}(t,\Delta) < \infty$?

$\mathrm{HeatContent}$ seams easier to study by methods of heat kernel analysis.

Theorem (van den Berg–Davies 1989)

If $\Omega \subset \mathbb{R}^d$ is horn-shaped and $t \geq 0$, then TFAE:

- $\mathrm{HeatTrace}_s(\Delta) < \infty$ *for all* $s > t$;
- $\mathrm{HeatContent}_s(\Delta) < \infty$ *for all* $s > t$.

Theorem (van den Berg–Gilkey 1994)

$$\mathrm{HeatContent}(t, \Delta) \asymp |\Omega| - \sum_{k=1}^{\infty} \beta_k t^{\frac{k}{2}} \qquad \text{as } t \to 0.$$

(many further results by van den Berg, Burchard, Caputo, Gilkey, Gittins, Kirsten, Miranda jr, Pallara, Paronetto, Rossi, Schmuckenschläger...)

On combinatorial graphs:

- $\mathrm{HeatTrace}$ since Stark–Terras 1996, Chung–Yau 1997
- $\mathrm{HeatContent}$ since McDonald–Meyers 2003

On metric graph:

- $\mathrm{HeatTrace}$ since Roth 1984
- $\mathrm{HeatContent}$ since Colladay–Kaganovskiy–McDonald 2017

The finite case

Spectral theory in the finite case ($\#E < \infty$)

$-\Delta^{\mathcal{G}}$ has pure point spectrum: its eigenvalues are

$$0 = \mu_1(\Delta^{\mathcal{G}}) < \mu_2(\Delta^{\mathcal{G}}) \leq \mu_3(\Delta^{\mathcal{G}}) \leq \ldots \nearrow \infty.$$

Theorem (Nicaise 1987; Band–Lévy 2017)

For any metric graph $\mathcal{G}$ on finitely many edges:

- $\mu_2(\Delta^{\mathcal{G}}) \geq \frac{\pi^2}{|\mathcal{G}|^2}$, *with equality iff* $\mathcal{G}=$

If additionally $\mathcal{G}$ is doubly connected, then

- $\mu_2(\Delta^{\mathcal{G}}) \geq \frac{4\pi^2}{|\mathcal{G}|^2}$, *with equality iff* $\mathcal{G}=$

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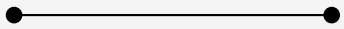
- $\mu_2(\Delta^{\mathcal{G}}) \ge \frac{\pi^2}{|\mathcal{G}|^2}$, *with equality iff* $\mathcal{G} =$ 

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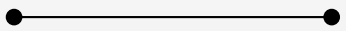
- $\mu_2(\Delta^{\mathcal{G}}) \geq \frac{\pi^2}{|\mathcal{G}|^2}$, *with equality iff* $\mathcal{G} =$ 

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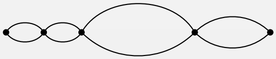
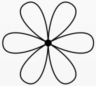
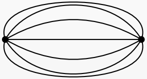
- $\mu_2(\Delta^{\mathcal{G}}) \geq \frac{4\pi^2}{|\mathcal{G}|^2}$, *with equality iff* $\mathcal{G} =$ 

Upper estimates

Theorem (Kennedy–Kurasov–Malenová–M. 2016; Band–Lévy 2017)
For any metric graph $\mathcal{G}$ on $E \geq 2$ edges:

- $\mu_2(\Delta^{\mathcal{G}}) \leq \frac{\pi^2 E^2}{|\mathcal{G}|^2}$, *with equality if* $\mathcal{G}=$  *or* $\mathcal{G}=$ 

  (but not only!, cf. Kurasov–Muller 2021, M.–Pivovarchik 2023)

If additionally $\mathcal{G}$ is a tree with E_l leaves, then

- $\mu_2(\Delta^{\mathcal{G}}) \leq \frac{\pi^2 E_l^2}{4|\mathcal{G}|^2}$ *with equality iff* $\mathcal{G}=$

Many, many more estimates in terms of diameter, inradius, Cheeger constant, first Betti number, length of cycles, avoidance diameter, mean distance, … by Amini, Berkolaiko, Exner, Kostenko, Nicolussi, Post, Rohleder, Solomyak …

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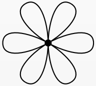
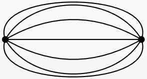
- $\mu_2(\Delta^{\mathcal{G}}) \leq \frac{\pi^2 E^2}{|\mathcal{G}|^2}$, *with equality if* $\mathcal{G}=$  *or* $\mathcal{G}=$ 

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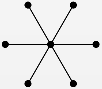
- $\mu_2(\Delta^{\mathcal{G}}) \leq \frac{\pi^2 E_l^2}{4|\mathcal{G}|^2}$ *with equality iff* $\mathcal{G}=$ 

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Dirichlet conditions

Upon imposing Dirichlet conditions on a vertex set $\emptyset \neq \mathsf{V}^{\mathrm{D}} \subset \mathsf{V}$, one may restrict $\mathfrak{a}$ to

$$H^1_0(\mathcal{G};\mathsf{V}^{\mathrm{D}}) := \{f \in H^1(\mathcal{G}) : f(\mathsf{v}) = 0 \ \forall \mathsf{v} \in \mathsf{V}^{\mathrm{D}}\}.$$

Again, consider the self-adjoint operator $\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}$ on $L^2(\mathcal{G})$ associated with $\big(\mathfrak{a}, H^1_0(\mathcal{G};\mathsf{V}^{\mathrm{D}})\big)$.

- $\big(\mathfrak{a}, H^1_0(\mathcal{G};\mathsf{V}^{\mathrm{D}})\big)$ is a Dirichlet form;
- If $\mathcal{G}$ has finitely many edges, $\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}$ has pure point spectrum with

$$0 < \lambda_1(\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) < \lambda_2(\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) \leq \lambda_3(\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) \ldots \nearrow \infty;$$

- $\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}$ is associated with a heat kernel $p^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}$ such that

$$0 \leq p_t^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}(x,y) \leq p_t^{\mathcal{G}}(x,y) \leq 1$$

Proposition

$$\int_{\mathcal{G}} p_t^{\mathcal{G}}(x,x)\,\mathrm{d}x \le \frac{|\mathcal{G}|}{\sqrt{4\pi t}} \quad \textit{and} \quad \liminf_{t\searrow 0} \sqrt{t}\int_{\mathcal{G}} p_t^{\mathcal{G};\mathrm{V^D}}(x,x)\,\mathrm{d}x \ge \frac{|\mathcal{G}|}{\sqrt{4\pi}}$$

Proof.

- Upper bound: Gaussian estimate satisfied by the heat kernels of $(\mathrm{e}^{t\Delta^{\mathcal{G}}})$ (M. 2007)
- Lower bound: Kac' "principle of not feeling the boundary" (Post–Rückriemen 2018)

□

Corollary (Nicaise 1987)

Weyl's law holds for $\Delta^{\mathcal{G}}$:

$$\lim_{k\to\infty} \frac{\mu_k(\Delta^{\mathcal{G}})}{k^2} = \lim_{k\to\infty} \frac{\lambda_k(\Delta^{\mathcal{G};\mathrm{V^D}})}{k^2} = \frac{\pi^2}{|\mathcal{G}|^2}$$

Proof.

Karamata's Tauberian Theorem

□

Geometric implications of Roth's formula: a heat content formula

Theorem (Bifulco–M. 2024)

$$\mathrm{HeatContent}(t, \Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) = |\mathcal{G}| - \frac{2\sqrt{t}}{\sqrt{\pi}}|\mathsf{V}^{\mathrm{D}}| + 4\sqrt{t} \sum_{\vec{p}\in\mathcal{P}_{\mathsf{V}^{\mathrm{D}}}(\mathcal{G})} \alpha(\vec{p})\, H\left(\frac{\mathrm{length}(\vec{p})}{2\sqrt{t}}\right)$$

for all $t > 0$.

- Here
$$H(x) := \frac{1}{\sqrt{\pi}}\mathrm{e}^{-x^2} - x\mathrm{erfc}(x)$$
for $\mathrm{erfc}(x) := \frac{2}{\sqrt{\pi}}\int_x^\infty \mathrm{e}^{-s^2}\,\mathrm{d}s$, $x \geq 0$; H maps $[0,\infty)$ to $[0,\infty)$ and is strictly monotonically decreasing, $0 \leq H(x) \lesssim \mathrm{e}^{-x^2}$;
- $\mathcal{P}_{\mathsf{V}^{\mathrm{D}}}(\mathcal{G})$ is the set of *all* (non-trivial) directed paths in $\mathcal{G}$ starting and ending at a vertex in V^{D}.

Sketch of the proof

Main steps:
1) Prove

$$\mathrm{HeatContent}(t, \Delta^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}) = |\mathcal{G}| + \frac{2\sqrt{t}}{\sqrt{\pi}}|\mathsf{E}| - 2\sqrt{t}\sum_{\mathsf{e}\in\mathsf{E}} H\left(\frac{\ell_{\mathsf{e}}}{2\sqrt{t}}\right)$$
$$+ \sqrt{t}\sum_{\vec{p}\in\mathcal{P}(\mathcal{G})} \alpha(\vec{p})\left(H\left(\frac{\ell(\vec{p})}{2\sqrt{t}}\right) - H\left(\frac{\ell(\vec{p}_-)}{2\sqrt{t}}\right) - H\left(\frac{\ell(\vec{p}_+)}{2\sqrt{t}}\right) + H\left(\frac{\ell(\vec{p}_\pm)}{2\sqrt{t}}\right)\right)$$

2) Use the strong decay properties of H to deduce that all these series are convergent: study them individually.
3) Analyze terms on the RHS: tedious combinatorial proof to find that sums over $\mathcal{P}(\mathcal{G})$ can be reduced to sums over $\mathcal{P}_{\mathrm{V}^{\mathrm{D}}}(\mathcal{G})$.
Key observation: Paths starting or ending at $\mathsf{V}\setminus\mathsf{V}^{\mathrm{D}}$ yield a vanishing contribution.

Small-time behavior of $\mathrm{HeatContent}(t,\Delta^{\mathcal{G}})$

Corollary

For all $0 < t < \frac{\ell_{\min}{}^2}{2\ln D_{\max}}$

$$\left|\mathrm{HeatContent}(t,\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) - |\mathcal{G}| + \frac{2\sqrt{t}}{\sqrt{\pi}}|\mathsf{V}^{\mathrm{D}}|\right| \le \frac{4\sqrt{t}}{\sqrt{\pi}\,d_{\max}} \frac{\mathrm{e}^{-\frac{\ell_{\min}^2}{4t}}}{1 - d_{\max}\mathrm{e}^{-\frac{\ell_{\min}^2}{2t}}}.$$

In particular: $\mathrm{HeatContent}(t,\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) \overset{t\to 0+}{\asymp} |\mathcal{G}| - \frac{2\sqrt{t}}{\sqrt{\pi}}|\mathsf{V}^{\mathrm{D}}| + \mathcal{O}\left(\sqrt{t}\mathrm{e}^{-\frac{\ell_{\min}^2}{4t}}\right)$

(to be compared with the small-time asymptotics by van den Berg–Gilkey!)

A Caccioppoli-type result

Theorem (Bifulco–M. 2024)

Let $\mathcal{H}$ be a subgraph of $\mathcal{G}$. Then

$$\lim_{t\to 0^+} \sqrt{\frac{\pi}{t}} \int_{\mathcal{H}} \int_{\mathcal{G}\setminus\mathcal{H}} p_t^{\mathcal{G}}(x,y)\,\mathrm{d}y\,\mathrm{d}x = |\partial\mathcal{H}|.$$

Similar result for $\Omega \subset \mathbb{R}^d$ under (very weak) geometric assumptions: Miranda–Pallara–Paronetto–Preunkert 2007.

Hadamard-type formula and surgery principles

Lemma (Bifulco–M. 2024)

Let $\mathcal{G}_s$, $s > 0$ be obtained from $\mathcal{G}$ by perturbing the length of an edge. Then

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=\ell_{\mathsf{e}_0}} \mathrm{HeatContent}(t, \Delta^{\mathcal{G}_s;\mathsf{V}^{\mathrm{D}}}) = 1 - 2 \sum_{\vec{p} \in \mathcal{P}_{\mathsf{V}^{\mathrm{D}}}(\mathcal{G})} \alpha(\vec{p}) |\vec{p}|_{\mathsf{e}_0} \mathrm{erfc}\left(\frac{\ell(\vec{p})}{2\sqrt{t}}\right), \qquad t > 0.$$

Lemma

If $\widetilde{\mathcal{G}}$ is obtained from $\mathcal{G}$

- *attaching a subgraph without Dirichlet vertices at a degree-1 vertex; or*
- *inserting an edge between adjacent edge; or*
- *mirroring $\mathcal{G}$ at some vertices in $\mathsf{V} \setminus \mathsf{V}^{\mathrm{D}}$; or*
- *cutting through the midpoint of a loop,*

then $\mathrm{HeatContent}(t, \Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) \le \mathrm{HeatContent}(t, \Delta^{\widetilde{\mathcal{G}};\mathsf{V}^{\mathrm{D}}})$

Outlook: Further self-adjoint extensions of Δ

Lemma (Kuchment 2003)

If $\mathcal{G}$ has $E<\infty$ edges, an extension of $\left(\Delta, \bigoplus_{e\in E} H^2_0(0,\ell_e)\right)$ on $L^2(\mathcal{G})$ is self-adjoint iff its domain is of the form

$$\left\{ f \in \bigoplus_{e\in E} H^2(0,\ell_e) : \underline{f} \in Y,\ \underline{\underline{f}} + R\underline{f} \in Y^\perp \right\}$$

for some $Y \leq \mathbb{C}^{4E}$ and some Hermitian $4E\times 4E$-matrix R.

Here

$$\underline{f} := \left(f_e(0), f_e(\ell_e)\right)_{e\in E}, \qquad \underline{\underline{f}} := \left(-f'_e(0), f'_e(\ell_e)\right)_{e\in E}$$

The extension *has no Robin part* if $R\equiv 0$.

Proposition (Kostrykin–Potthoff–Schrader 2007)

Roth's formula extends to general self-adjoint extensions with no Robin part.

Proposition (Cardanobile–M. 2008)

The quadratic form associated with a self-adjoint extension with no Robin part is a Dirichlet form iff the orthogonal projector of $\mathbb{C}^{4E}$ onto Y is Markovian.

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The only other known exact formula: trace formula

Theorem (Roth 1984; Nicaise 1987; Kostrykin–Potthoff–Schrader 2007)

For a $\mathcal{G}$ with V vertices (V_D of them Dirichlet) and E edges:

- *pure standard conditions:*

$$\int_{\mathcal{G}} p_t^{\mathcal{G}}(x,x)\,\mathrm{d}x = \frac{|\mathcal{G}|}{\sqrt{4\pi t}} + \frac{V-E}{2} + \frac{1}{\sqrt{4\pi t}} \sum_C \alpha(C)\mathrm{length}(\tilde{C})\mathrm{e}^{-\frac{\mathrm{length}(C)^2}{4t}}$$

- *Dirichlet conditions at* V^{D}*:*

$$\int_{\mathcal{G}} p_t^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}(x,x)\,\mathrm{d}x = \frac{|\mathcal{G}|}{\sqrt{4\pi t}} + \frac{V-V_D-E}{2} + \frac{1}{\sqrt{4\pi t}} \sum_C \alpha(C)\mathrm{length}(\tilde{C})\mathrm{e}^{-\frac{\mathrm{length}(C)^2}{4t}}$$

- *general self-adjoint conditions with no Robin part, scattering matrix* $\mathfrak{S}$*:*

$$\int_{\mathcal{G}} p_t^{\mathcal{G};\mathfrak{S}}(x,x)\,\mathrm{d}x = \frac{|\mathcal{G}|}{\sqrt{4\pi t}} + \mathrm{tr}(\mathfrak{S}) + \frac{1}{\sqrt{4\pi t}} \sum_C \alpha(C)\mathrm{length}(\tilde{C})\mathrm{e}^{-\frac{\mathrm{length}(C)^2}{4t}}$$

All these formulae hold *for all* $t > 0$!

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$$\int_{\mathcal{G}} p_t^{\mathcal{G}}(x,x)\,\mathrm{d}x = \frac{|\mathcal{G}|}{\sqrt{4\pi t}} + \frac{V-E}{2} + \frac{1}{\sqrt{4\pi t}} \sum_C \alpha(C)\mathrm{length}(\tilde{C})\mathrm{e}^{-\frac{\mathrm{length}(C)^2}{4t}}$$

- *Dirichlet conditions at* V^{D}*:*

$$\int_{\mathcal{G}} p_t^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}(x,x)\,\mathrm{d}x = \frac{|\mathcal{G}|}{\sqrt{4\pi t}} + \frac{V-V_D-E}{2} + \frac{1}{\sqrt{4\pi t}} \sum_C \alpha(C)\mathrm{length}(\tilde{C})\mathrm{e}^{-\frac{\mathrm{length}(C)^2}{4t}}$$

- *general self-adjoint conditions with no Robin part, scattering matrix* $\mathfrak{S}$*:*

$$\int_{\mathcal{G}} p_t^{\mathcal{G};\mathfrak{S}}(x,x)\,\mathrm{d}x = \frac{|\mathcal{G}|}{\sqrt{4\pi t}} + \mathrm{tr}(\mathfrak{S}) + \frac{1}{\sqrt{4\pi t}} \sum_C \alpha(C)\mathrm{length}(\tilde{C})\mathrm{e}^{-\frac{\mathrm{length}(C)^2}{4t}}$$

All these formulae hold *for all* $t > 0$!

The bounded geometry case

Proposition (Becker–Gregorio–M. 2021)

$\Delta + V$ generates a positivity improving semigroup on all $L^p(\mathcal{G})$ and on $C_0(\mathcal{G})$, $BUC(\mathcal{G})$ for any $V \in L^\infty(\mathcal{G})$.

Proposition (Becker–Gregorio–M. 2021)

If the volume grows sub-exponentially, 0 is a simple eigenvalue of the $BUC(\mathcal{G})$-realization of $\Delta^{\mathcal{G}}$.
Away from the point spectrum and the Dirichlet spectrum, the continuous spectrum of $\Delta^{\mathcal{G}}$ on $L^p(\mathcal{G})$, $C_0(\mathcal{G})$ or $BUC(\mathcal{G})$ can be characterized in terms of transition matrices of random walks of infinite graphs in appropriate sequence spaces.

Proposition (Becker–Gregorio–M. 2021)

The spectrum of $\Delta^{\mathcal{G}}$ on $L^p(\mathcal{G})$ is p-independent.
A Feynman–Kac formula holds and a Gaussian-like estimate holds if $V \in C(\mathcal{G}) \cap L^\infty(\mathcal{G})$.

The unbounded geometry case

Given an infinite, locally finite $\mathcal{G}$:
Consider the operator $\Delta^{\mathcal{G}}_{\text{min}}$ on $L^2(\mathcal{G})$ associated with the closable Dirichlet form

$$\mathfrak{a}(f) := \int_{\mathcal{G}} |f'|^2 \,\mathrm{d}x$$

$$\mathrm{dom}_{min}(\mathfrak{a}) := \{f \in H^1(\mathcal{G}) : f \text{ finitely supported}\}$$

Exner–Kostenko–Malamud–Neidhardt 2018: Essential self-adjointness of $\Delta^{\mathcal{G}}_{\text{min}}$ is related to essential self-adjointness of a weighted discrete Laplacian.

Kostenko–Nicolussi 2019: Spectral analysis of the Friedrichs extension of $\Delta^{\mathcal{G}}_{\text{min}}$.

Definition

Consider sequences $\mathcal{U} = (U_n)$ of nonempty open connected subsets of $\mathcal{G}$ with compact boundaries such that

$$\dots U_{n+1} \subset U_n \subset U_{n-1} \dots \quad \textit{and} \quad \bigcap_{n\in\mathbb{N}} \overline{U_n} = \emptyset.$$

$\mathcal{U} = (U_n)$ and $\mathcal{U}' = (U_n')$ are **equivalent** *if for all $n \in \mathbb{N}$ there exist j, k, such that $U_j' \subset U_n$ and $U_k \subset U_n'$.*
An equivalence class γ of sequences is called an **end** *of $\mathcal{G}$.*
γ has **finite volume** *if $|U_n| < \infty$ for some n.*

Example

- $\mathbb{Z}$ has two ends: $\{+\infty, -\infty\}$
- $\mathbb{Z}^2$ has one end: $\{\infty\}$
- the binary tree has uncountably many ends: $\simeq [0, 1]$

An isoperimetric inequality for infinite metric graphs

Theorem (Carlson 2000; Düfel–Kennedy–M.–Plümer–Täufer 2023)
$\Delta^{\mathcal{G}}$ has compact resolvent if $|\mathcal{G}| < \infty$; in this case, $\mu_2(\Delta^{\mathcal{G}}) \geq \frac{\pi^2}{|\mathcal{G}|^2}$, with equality iff $\mathcal{G} =$ 

Ali Mehmeti–Nicaise 1993, Solomyak 2004, Kostenko–Nicolussi 2019:
$\Delta^{\mathcal{G}}$ may have purely discrete spectrum even though $|\mathcal{G}| = \infty$!

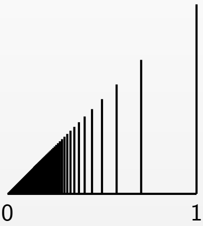
Theorem (Kostenko–M.–Nicolussi 2022)

If $|\mathcal{G}| < \infty$ and if (!) the domain of $\Delta^{\mathcal{G}}$ is contained in $H^1(\mathcal{G})$, then $\Delta^{\mathcal{G}}$ is associated with a heat kernel and the generated semigroup is of trace class.

- A Roth-type kernel formula is unknown.
- No trace formula is known.
- No heat content formula is known.

A class of more sophisticated examples

For $\alpha > 0$, introduce the **diagonal comb graph** $\mathcal{G}_\alpha$ by taking the interval $(0,1]$, putting a vertex at $\frac{1}{n^\alpha}$, $n \in \mathbb{N}$, and attaching to it an edge of length $\frac{1}{n^\alpha}$.



By **Kostenko–M.–Nicolussi 2022**: 0 is the only end and

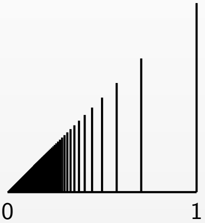
- either $|\mathcal{G}_\alpha| = \infty$ and $\Delta^{\mathcal{G}_\alpha}$ is essentially self-adjoint;
- or $|\mathcal{G}_\alpha| < \infty$ and the deficiency index of $\Delta^{\mathcal{G}_\alpha}$ is 1: we impose a Neumann condition at the end.

$\alpha > 1 \Leftrightarrow |\mathcal{G}_\alpha| < \infty \Rightarrow \Delta^{\mathcal{G}_\alpha}$ has pure point spectrum.

Phase transition in the spectrum of comb graphs

Theorem (Düfel–Kennedy–M.–Plümer–Täufer 2023)

1. *For all $\alpha > \frac{1}{2}$, $\Delta^{\mathcal{G}_\alpha}$ has pure point spectrum.*
2. *For all $\alpha \in (0, \frac{1}{2}]$, $\Delta^{\mathcal{G}_\alpha}$ has nonempty essential spectrum.*



Proof.

1. Kolmogorov–Riesz-type compactness theorem
2. Explicit construction of a Weyl sequence: $\inf \sigma(\Delta^{\mathcal{G}_\alpha}) = 0$ for $\alpha \in (0, \frac{1}{2})$. $\square$

Non-Weyl asymptotics

Proposition (Kennedy–M.–Täufer 2024)

The eigenvalues of $\Delta^{\mathcal{G}_\alpha}$ satisfy

- *for all $\alpha \in (\frac{1}{2}, 1)$: for j large enough*

$$c_\alpha j^{4\alpha-2} \leq \lambda_j(\mathcal{G}_\alpha) \leq C_\alpha j^{2\alpha}$$

- *for $\alpha = 1$: for j large enough*

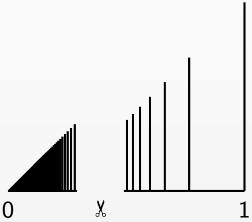
$$c\left(\frac{j}{(\log j)^2}\right)^2 \leq \lambda_j(\mathcal{G}_1) \leq C\left(\frac{j}{\log j}\right)^2$$

- *for $\alpha > 1$: for $j \geq 2$*

$$\frac{j^2\pi^2}{4|\mathcal{G}_\alpha|^2} \leq \lambda_j(\mathcal{G}_\alpha) \leq \frac{j^2\pi^2}{4}$$

Examples of non-Weyl asymptotics already known for quantum graphs on fractals: Alonso-Ruiz–Freiberg 2017, wrt *non-Lebesgue* measure.

Proof.



- Split the graph in a sparse part of finite volume and a dense part of small mean distance.
- Apply known upper/lower estimates for eigenvalues of metric trees (**Berkolaiko–Kennedy–Kurasov–M. 2017**)
- Use domain monotonicity.

□

Torsional geometry

Torsion of metric graphs

Let

$$\sup_{u\in H^1_0(\mathcal{G};\mathsf{V}_D)} \frac{\left(\int_{\mathcal{G}} u\,\mathrm{d}x\right)^2}{\|u'\|^2_{L^2}} =: T(\Delta^{\mathcal{G};\mathrm{V}^{\mathrm{D}}});$$

the maximizer is the **torsion function** of $\mathcal{G}$, i.e., the only solution on

$$\begin{cases} -\Delta v(x) = 1, & x \in \mathcal{G}, \\ v(\mathsf{v}) = 0, & \mathsf{v} \in \mathsf{V}_D, \end{cases}$$

and

$$T(\mathcal{G};\mathsf{V}_D) = \|v\|_{L^1}$$

is called **torsional rigidity** of $\mathcal{G}$ wrt V^{D}.
Observe: $v(x) = \int_0^\infty \mathrm{e}^{t\Delta_{\mathcal{G}}}\mathbb{1}(x)\,\mathrm{d}x$, hence

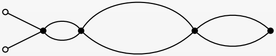
$$T(\Delta^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}) = \int_0^\infty \mathrm{HeatContent}(t, \Delta^{\mathcal{G};\mathrm{V}^{\mathrm{D}}})\,\mathrm{d}t.$$

Theorem (Mondino–Vedovato 2021; M.–Plümer 2023)

For any metric graph $\mathcal{G}$ on finitely many edges:

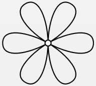
- $T(\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) \leq \frac{|\mathcal{G}|^3}{3}$, *with equality iff* $\mathcal{G}=$ 

If additionally $\mathcal{G}$ is doubly connected, then

- $T(\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) \leq \frac{|\mathcal{G}|^3}{12}$, *with equality iff* $\mathcal{G}=$ 

Theorem (M.–Plümer 2023)

For any metric graph $\mathcal{G}$ on finitely many edges:

- $T(\Delta^{\mathcal{G};\mathsf{V}^{\mathrm{D}}}) \geq \frac{1}{12}\frac{|\mathcal{G}|^3}{|\mathsf{E}|^3}$ *with equality iff* $\mathcal{G}=$ 

Saint-Venant and Kohler-Jobin inequalities

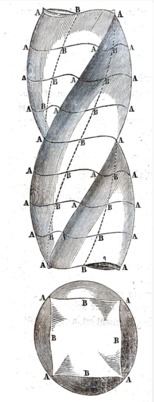


Figure: A.J.C.B. de Saint-Venant 1856

$$T(\Omega) := \sup_{u \in H_0^1(\Omega)} \frac{\left(\int_\Omega u \, \mathrm{d}x\right)^2}{\|\nabla u\|_{L^2}^2}$$

Theorem (Pólya 1948; Pólya–Weinstein 1950)

Among all bounded, open domains $\Omega \subset \mathbb{R}^d$ of given (finite) volume, $T(\Omega)$ is maximized by the ball.

Among all bounded, open, not simply connected domains $\Omega \subset \mathbb{R}^d$ of given (finite) volume and given combined volume of the holes, $T(\Omega)$ is maximized by the annulus.

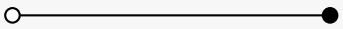
Theorem (Kohler-Jobin 1978; Brasco 2013)

Among all open domains $\Omega \subset \mathbb{R}^d$ of given (finite) volume, $\lambda_1(\Omega) T^{\frac{2}{2+d}}(\Omega)$ is minimized by the ball, and only by it.

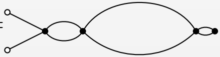
Kohler-Jobin inequality on metric graphs

Theorem (M.–Plümer 2023)

For any metric graph $\mathcal{G}$ on finitely many edges:

- $\left(\frac{\pi}{\sqrt[3]{24}}\right)^2 \leq \lambda_1(\mathcal{G};\mathsf{V}_D)T(\mathcal{G};\mathsf{V}_D)^{\frac{2}{3}}$, *with equality iff* $\mathcal{G}=$ 

If additionally $\mathcal{G}$ is doubly connected, then:

- $\left(\frac{\pi}{\sqrt[3]{12}}\right)^2 \leq \lambda_1(\mathcal{G};\mathsf{V}_D)T(\mathcal{G};\mathsf{V}_D)^{\frac{2}{3}}$, *with equality iff* $\mathcal{G}=$ 

Schwarz/Steiner symmetrization will not work!

Thank you for your attention!

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