Diffusion problems on metric graphs

Delio Mugnolo

University of Hagen

CIMPA School 2025
Transport optimal, EDP et optimisation applications en sciences des données

May 2025

$$
\begin{cases}
\dfrac{\partial u}{\partial t}(t,x) = \Delta u(t,x) & t \geq 0,\ x \in \Omega, \\
u(t,z) = 0 & t \geq 0,\ z \in \partial\Omega, \\
u(0,x) = u_0(x) & x \in \Omega.
\end{cases}
$$

If $\Omega \subset \mathbb{R}^d$ is open bounded, $\partial\Omega$ smooth, then Δ with Dirichlet BCs is self-adjoint and negative semidefinite, and it has compact resolvent:

- the eigenvalues λ_k, $k \in \mathbb{N}$, of $-\Delta$ have finite multiplicities and accumulate at $+\infty$
- there exists an ONB of $L^2(\Omega)$ consisting of corresponding eigenfunctions φ_k, $k \in \mathbb{N}$.

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \Delta u(t,x) & t \geq 0,\ x \in \Omega, \\ u(t,z) = 0 & t \geq 0,\ z \in \partial\Omega, \\ u(0,x) = u_0(x) & x \in \Omega. \end{cases}$$

If $\Omega \subset \mathbb{R}^d$ is open bounded, $\partial\Omega$ smooth, then Δ with Dirichlet BCs is self-adjoint and negative semidefinite, and it has compact resolvent:

- the eigenvalues λ_k, $k \in \mathbb{N}$, of $-\Delta$ have finite multiplicities and accumulate at $+\infty$
- there exists an ONB of $L^2(\Omega)$ consisting of corresponding eigenfunctions φ_k, $k \in \mathbb{N}$.

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \Delta u(t,x) & t \geq 0,\ x \in \Omega, \\ u(t,z) = 0 & t \geq 0,\ z \in \partial\Omega, \\ u(0,x) = u_0(x) & x \in \Omega. \end{cases}$$

If $\Omega \subset \mathbb{R}^d$ is open bounded, $\partial\Omega$ smooth, then Δ with Dirichlet BCs is self-adjoint and negative semidefinite, and it has compact resolvent:

- the eigenvalues λ_k, $k \in \mathbb{N}$, of $-\Delta$ have finite multiplicities and accumulate at $+\infty$
- there exists an ONB of $L^2(\Omega)$ consisting of corresponding eigenfunctions φ_k, $k \in \mathbb{N}$.

Solving by Fourier transformation

By Spectral Theorem + elementary functional calculus

$$
\begin{aligned}
u(t,x) &= \mathrm{e}^{t\Delta} u_0(x) \\
&= \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} \langle \varphi_k, u_0 \rangle_{L^2(\Omega)} \varphi_k(x) \\
&\overset{\triangle!}{=} \int_\Omega \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} \varphi_k(x)\varphi_k(y) u_0(y)\,\mathrm{d}y \\
&=: \int_\Omega p_t(x,y) u_0(y)\,\mathrm{d}y
\end{aligned}
$$

Is this legit?

Solving by Fourier transformation

By Spectral Theorem + elementary functional calculus

$$u(t,x) = \mathrm{e}^{t\Delta} u_0(x)$$
$$= \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} \langle \varphi_k, u_0 \rangle_{L^2(\Omega)} \varphi_k(x)$$
$$\overset{\triangle!}{=} \int_\Omega \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} \varphi_k(x)\varphi_k(y) u_0(y)\,\mathrm{d}y$$
$$=: \int_\Omega p_t(x,y) u_0(y)\,\mathrm{d}y$$

Is this legit?

Solving by Fourier transformation

By Spectral Theorem + elementary functional calculus

$$
\begin{aligned}
u(t,x) &= \mathrm{e}^{t\Delta} u_0(x) \\
&= \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} \langle \varphi_k, u_0 \rangle_{L^2(\Omega)} \varphi_k(x) \\
&\overset{\triangle!}{=} \int_\Omega \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} \varphi_k(x)\varphi_k(y) u_0(y)\,\mathrm{d}y \\
&=: \int_\Omega p_t(x,y) u_0(y)\,\mathrm{d}y
\end{aligned}
$$

Is this legit?

Mercer's Theorem

James Mercer
1883–1932

Theorem (Mercer 1909)

Let $\Omega \subset \mathbb{R}^d$ bounded, and let $k \in C(\overline{\Omega} \times \overline{\Omega})$ be a symmetric **kernel** *such that*

$$T_k : f \mapsto \int_\Omega k(x,y) f(y) \, \mathrm{d}\mu(y)$$

is positive semidefinite on $L^2(\Omega)$. Let $(\varphi_n)_{n\in\mathbb{N}}$ be an ONB of eigenvectors of T_k with eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$. Then

- $(\lambda_n)_{n\in\mathbb{N}} \in \ell^1$;
- *the series*

$$\sum_{n\in\mathbb{N}} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

  converges absolutely and uniformly in $\|(\cdot,\cdot)\|_\infty$ for all $(x,y) \in \Omega \times \Omega$...
- *...and it agrees with $k(x,y)$.*

Mercer's Theorem

James Mercer

1883–1932

Theorem (Mercer 1909)

Let $\Omega \subset \mathbb{R}^d$ bounded, and let $k \in C(\overline{\Omega} \times \overline{\Omega})$ be a symmetric **kernel** *such that*

$$T_k : f \mapsto \int_\Omega k(x,y) f(y) \, \mathrm{d}\mu(y)$$

is positive semidefinite on $L^2(\Omega)$. Let $(\varphi_n)_{n\in\mathbb{N}}$ be an ONB of eigenvectors of T_k with eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$. Then

- $(\lambda_n)_{n\in\mathbb{N}} \in \ell^1$;
- *the series*

  $$\sum_{n\in\mathbb{N}} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

  converges absolutely and uniformly in $\|(\cdot,\cdot)\|_\infty$ for all $(x,y) \in \Omega \times \Omega$...
- *...and it agrees with $k(x,y)$.*

Mercer's Theorem revisited

Theorem (Mercer 1909; König 1986)

Let $\Omega \subset \mathbb{R}^d$ bounded, and let $k \in L^\infty(\Omega \times \Omega)$ be a **kernel** *such that*

$$T_k : f \mapsto \int_\Omega k(x,y) f(y) \, \mathrm{d}\mu(y)$$

is positive semidefinite on $L^2(\Omega)$. Let $(\varphi_n)_{n\in\mathbb{N}}$ be an ONB of eigenvectors of T_k with eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$ s.t. $\sup_{n\in\mathbb{N}} \|\varphi_n\|_\infty \le C$ for some $C > 0$. Then

- $(\lambda_n)_{n\in\mathbb{N}} \in \ell^1$;
- *the series*

$$\sum_{n\in\mathbb{N}} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

  converges absolutely and uniformly in $\|(\cdot,\cdot)\|_\infty$ for $\mu \otimes \mu$-a.e. $(x,y) \in \Omega \times \Omega$...
- *...and it agrees with $k(x,y)$ for $\mu \otimes \mu$-a.e. $(x,y) \in \Omega \times \Omega$.*

⚠

Wrong in König's book! (formulated under too weak assumptions: counterexamples exist)

This version is correct.

Mercer's Theorem revisited

Theorem (Mercer 1909; König 1986)

Let $\Omega \subset \mathbb{R}^d$ bounded, and let $k \in L^\infty(\Omega \times \Omega)$ be a **kernel** *such that*

$$T_k : f \mapsto \int_\Omega k(x,y) f(y) \, \mathrm{d}\mu(y)$$

is positive semidefinite on $L^2(\Omega)$. Let $(\varphi_n)_{n\in\mathbb{N}}$ be an ONB of eigenvectors of T_k with eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$ s.t. $\sup_{n\in\mathbb{N}} \|\varphi_n\|_\infty \le C$ for some $C > 0$. Then

- $(\lambda_n)_{n\in\mathbb{N}} \in \ell^1$;
- *the series*

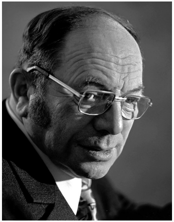
  $$\sum_{n\in\mathbb{N}} \lambda_n \varphi_n(x) \overline{\varphi_n(y)}$$

  converges absolutely and uniformly in $\|(\cdot,\cdot)\|_\infty$ for $\mu \otimes \mu$-a.e. $(x,y) \in \Omega \times \Omega$...
- *...and it agrees with $k(x,y)$ for $\mu \otimes \mu$-a.e. $(x,y) \in \Omega \times \Omega$.*

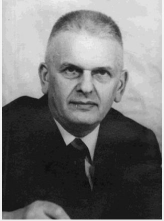
⚠
Wrong in König's book! (formulated under too weak assumptions: counterexamples exist)

This version is correct.

Kantorovič–Wulich Theorem



Leonid Vital'evič Kantorovič
1912–1986



Boris Sacharowitsch Wulich
1913–1978

Theorem (Kantorovič–Wulich 1937)

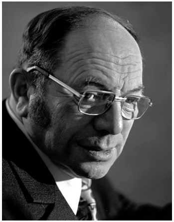
Let $p \in [1, \infty)$, and let $(\Omega; \mu)$ be any σ-finite measure space. Any operator in $\mathcal{L}(L^p(\Omega); L^\infty(\Omega))$ is an integral operator with kernel of class $L^\infty(\Omega; L^{p'}(\Omega))$, and vice versa.

Corollary

Let T be a self-adjoint operator that is bounded from $L^1(\Omega)$ to $L^2(\Omega)$.

- *$T^* T$ is an integral operator with kernel of class $L^\infty(\Omega \times \Omega)$.*
- *If Ω has finite measure, then $T^* T$ is a Hilbert–Schmidt operator.*

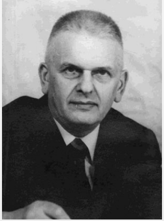
Kantorovič–Wulich Theorem



Leonid Vital'evič Kantorovič
1912–1986

Theorem (Kantorovič–Wulich 1937)

Let $p \in [1, \infty)$, and let $(\Omega; \mu)$ be any σ-finite measure space. Any operator in $\mathcal{L}(L^p(\Omega); L^\infty(\Omega))$ is an integral operator with kernel of class $L^\infty(\Omega; L^{p'}(\Omega))$, and vice versa.



Boris Sacharowitsch Wulich
1913–1978

Corollary

Let T be a self-adjoint operator that is bounded from $L^1(\Omega)$ to $L^2(\Omega)$.

- *T^*T is an integral operator with kernel of class $L^\infty(\Omega \times \Omega)$.*
- *If Ω has finite measure, then T^*T is a Hilbert–Schmidt operator.*

Back to the heat equation!

- $e^{t\Delta}$ is compact, self-adjoint, and positive definite, bounded from $L^2(\Omega)$ to $L^\infty(\Omega)$, hence ($e^{t\Delta} = e^{\frac{t}{2}\Delta}e^{\frac{t}{2}\Delta}$) from $L^1(\Omega)$ to $L^\infty(\Omega)$.
- Kantorovič–Wulich: $\rightsquigarrow p_t \in L^\infty(\Omega \times \Omega)$.
- Arendt:
$$p_t(x,y) = \sum_{k\in\mathbb{N}} e^{-t\lambda_k}\varphi_k(x)\varphi_k(y)$$
converges absolutely and uniformly in $\|(\cdot,\cdot)\|_\infty$, for all $t > 0$ and all $(x,y) \in \Omega \times \Omega$.
- $e^{t\Delta}$ is of trace class $\forall t > 0$ and $\sup_k \|\varphi_k\|_\infty < \infty$.

$p = p_t(x,y)$ is the **heat kernel**:

Knowing p suffices to find a solution of

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \Delta u(t,x) & t \geq 0,\ x \in \Omega, \\ u(t,z) = 0 & t \geq 0,\ z \in \partial\Omega, \\ u(0,x) = u_0(x) & x \in \Omega. \end{cases}$$

for all $u_0 \in L^2(\Omega)$.

How do kernels work?

- If $A = (a_{ij})$ is $n \times n$ matrix and T_A the associated linear transformation, then

$$(T_A\xi)_i = \sum_{j=1}^{n} a_{ij}\xi_j \equiv \int_{\{1,\ldots,n\}} a(i,j)\xi(j)\,\mathrm{d}\mu(j)$$

  i.e., A is the kernel of T_A. So $T_A\xi \equiv A\xi$.

- If A is Hermitian, then there is a change of basis $U : e_k \leftrightarrow \varphi_k$ such that

$$U^*AU = \mathrm{diag}(\lambda_k), \quad \text{i.e.,} \quad T_A\xi \equiv A\xi = \sum_{k=1}^{n} \lambda_k\langle\xi,\varphi_k\rangle\varphi_k$$

- The linear, finite dimensional dynamical system

$$\begin{cases} \dot{\xi}(t) = A\xi(t) & t \geq 0, \\ \xi(0) = \xi_0 \end{cases}$$

  is solved by $\xi(t) = \mathrm{e}^{tA}\xi_0$, i.e.,

$$\xi_i(t) = \sum_{j=1}^{n} (\mathrm{e}^{tA})_{ij}\xi_{0,j} \equiv \int_{\{1,\ldots,n\}} \mathrm{e}^{tA}(i,j)\xi_0(j)\,\mathrm{d}\mu(j)$$

- *Heat* kernels of finite dimensional dynamical systems?

How do kernels work?

- If $A = (a_{ij})$ is $n \times n$ matrix and T_A the associated linear transformation, then

$$(T_A\xi)_i = \sum_{j=1}^{n} a_{ij}\xi_j \equiv \int_{\{1,\dots,n\}} a(i,j)\xi(j)\,\mathrm{d}\mu(j)$$

i.e., A is the kernel of T_A. So $T_A\xi \equiv A\xi$.

- If A is Hermitian, then there is a change of basis $U : e_k \leftrightarrow \varphi_k$ such that

$$U^*AU = \mathrm{diag}(\lambda_k), \quad \text{i.e.,} \quad T_A\xi \equiv A\xi = \sum_{k=1}^{n} \lambda_k\langle\xi,\varphi_k\rangle\varphi_k$$

- The linear, finite dimensional dynamical system

$$\begin{cases} \dot{\xi}(t) = A\xi(t) & t \geq 0, \\ \xi(0) = \xi_0 \end{cases}$$

is solved by $\xi(t) = \mathrm{e}^{tA}\xi_0$, i.e.,

$$\xi_i(t) = \sum_{j=1}^{n} (\mathrm{e}^{tA})_{ij}\xi_{0,j} \equiv \int_{\{1,\dots,n\}} \mathrm{e}^{tA}(i,j)\xi_0(j)\,\mathrm{d}\mu(j)$$

- *Heat* kernels of finite dimensional dynamical systems?

How do kernels work?

- If $A = (a_{ij})$ is $n \times n$ matrix and T_A the associated linear transformation, then

$$(T_A\xi)_i = \sum_{j=1}^{n} a_{ij}\xi_j \equiv \int_{\{1,\ldots,n\}} a(i,j)\xi(j)\,\mathrm{d}\mu(j)$$

  i.e., A is the kernel of T_A. So $T_A\xi \equiv A\xi$.

- If A is Hermitian, then there is a change of basis $U : e_k \leftrightarrow \varphi_k$ such that

$$U^*AU = \mathrm{diag}(\lambda_k), \quad \text{i.e.,} \quad T_A\xi \equiv A\xi = \sum_{k=1}^{n} \lambda_k \langle \xi, \varphi_k \rangle \varphi_k$$

- The linear, finite dimensional dynamical system

$$\begin{cases} \dot{\xi}(t) = A\xi(t) & t \geq 0, \\ \xi(0) = \xi_0 \end{cases}$$

  is solved by $\xi(t) = \mathrm{e}^{tA}\xi_0$, i.e.,

$$\xi_i(t) = \sum_{j=1}^{n} (\mathrm{e}^{tA})_{ij}\xi_{0,j} \equiv \int_{\{1,\ldots,n\}} \mathrm{e}^{tA}(i,j)\xi_0(j)\,\mathrm{d}\mu(j)$$

- *Heat* kernels of finite dimensional dynamical systems?

How do kernels work?

- If $A = (a_{ij})$ is $n \times n$ matrix and T_A the associated linear transformation, then

$$(T_A \xi)_i = \sum_{j=1}^{n} a_{ij} \xi_j \equiv \int_{\{1,\dots,n\}} a(i,j)\xi(j)\,\mathrm{d}\mu(j)$$

  i.e., A is the kernel of T_A. So $T_A \xi \equiv A\xi$.

- If A is Hermitian, then there is a change of basis $U : e_k \leftrightarrow \varphi_k$ such that

$$U^* AU = \mathrm{diag}(\lambda_k), \quad \text{i.e.,} \quad T_A \xi \equiv A\xi = \sum_{k=1}^{n} \lambda_k \langle \xi, \varphi_k \rangle \varphi_k$$

- The linear, finite dimensional dynamical system

$$\begin{cases} \dot{\xi}(t) = A\xi(t) & t \geq 0, \\ \xi(0) = \xi_0 \end{cases}$$

  is solved by $\xi(t) = \mathrm{e}^{tA}\xi_0$, i.e.,

$$\xi_i(t) = \sum_{j=1}^{n} (\mathrm{e}^{tA})_{ij} \xi_{0,j} \equiv \int_{\{1,\dots,n\}} \mathrm{e}^{tA}(i,j)\xi_0(j)\,\mathrm{d}\mu(j)$$

- *Heat* kernels of finite dimensional dynamical systems?

How do kernels work?

- If $A = (a_{ij})$ is $n \times n$ matrix and T_A the associated linear transformation, then

$$(T_A\xi)_i = \sum_{j=1}^{n} a_{ij}\xi_j \equiv \int_{\{1,\dots,n\}} a(i,j)\xi(j)\,\mathrm{d}\mu(j)$$

  i.e., A is the kernel of T_A. So $T_A\xi \equiv A\xi$.

- If A is Hermitian, then there is a change of basis $U : e_k \leftrightarrow \varphi_k$ such that

$$U^*AU = \mathrm{diag}(\lambda_k), \quad \text{i.e.,} \quad T_A\xi \equiv A\xi = \sum_{k=1}^{n} \lambda_k \langle \xi, \varphi_k \rangle \varphi_k$$

- The linear, finite dimensional dynamical system

$$\begin{cases} \dot{\xi}(t) = A\xi(t) & t \geq 0, \\ \xi(0) = \xi_0 \end{cases}$$

  is solved by $\xi(t) = \mathrm{e}^{tA}\xi_0$, i.e.,

$$\xi_i(t) = \sum_{j=1}^{n} (\mathrm{e}^{tA})_{ij}\xi_{0,j} \equiv \int_{\{1,\dots,n\}} \mathrm{e}^{tA}(i,j)\xi_0(j)\,\mathrm{d}\mu(j)$$

- *Heat* kernels of finite dimensional dynamical systems?

Kernel trick

- If $A = (a_{ij})$ is a stochastic matrix, i.e., A is positive and $A\mathbb{1} = \mathbb{1}$, then $0 \leq a_{ij} \leq 1$ and $\sum_j a_{ij} = 1$.
- Therefore, each $(a_{ij})_j$ can be regarded as a **probability distribution**: the larger a_{ij}, the more akin i, j.
- i, j are just numbers! or perhaps features of inputs in a general data set.
- Idea! Compare $\mathbf{x}, \mathbf{y}$ by
  - mapping them to numbers $i_{\mathbf{x}}, j_{\mathbf{y}} \in \{1, \ldots, n\}$,
  - then estimating their kinship via $a_{i_{\mathbf{x}}, j_{\mathbf{y}}}$.
- Can do the same for general kernel p of positive semidefinite, Markovian integral operator (but $p(x, y) > 1$ is possible!, stay tuned).

Kernel trick

- If $A = (a_{ij})$ is a stochastic matrix, i.e., A is positive and $A\mathbb{1} = \mathbb{1}$, then $0 \leq a_{ij} \leq 1$ and $\sum_j a_{ij} = 1$.
- Therefore, each $(a_{ij})_j$ can be regarded as a **probability distribution**: the larger a_{ij}, the more akin i, j.
- i, j are just numbers! or perhaps features of inputs in a general data set.
- Idea! Compare $\mathbf{x}, \mathbf{y}$ by
  - mapping them to numbers $i_\mathbf{x}, j_\mathbf{y} \in \{1, \ldots, n\}$,
  - then estimating their kinship via $a_{i_\mathbf{x}, j_\mathbf{y}}$.
- Can do the same for general kernel p of positive semidefinite, Markovian integral operator (but $p(x, y) > 1$ is possible!, stay tuned).

Heat kernel trick?

- Let $A = (a_{ij})$ be a matrix s.t. e^{tA} is stochastic for all t.
- Study a *family* of kernels e^{tA}, $t \in \mathbb{R}$.
- $\mathrm{e}^{0A} = \mathrm{Id}$: each object is only akin to itself only.
- $\mathrm{e}^{tA} \overset{t\to\infty}{\to} P_{\ker(A)}$: e.g., any two objects are akin. [1]
- In general, e^{tA} will smoothly interpolate between these behaviors, depending on $t \equiv$ inverse temperature.

[1] e^{tA} stochastic $\Rightarrow \ker(A) = \langle \mathbb{1} \rangle$

Heat kernel trick?

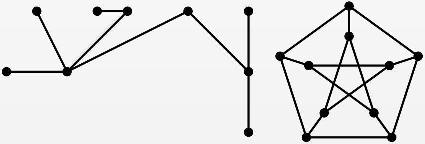
- Let $A = (a_{ij})$ be a matrix s.t. e^{tA} is stochastic for all t.
- Study a *family* of kernels e^{tA}, $t \in \mathbb{R}$.
- $\mathrm{e}^{0A} = \mathrm{Id}$: each object is only akin to itself only.
- $\mathrm{e}^{tA} \stackrel{t\to\infty}{\to} P_{\ker(A)}$: e.g., any two objects are akin. [1]
- In general, e^{tA} will smoothly interpolate between these behaviors, depending on $t \equiv$ inverse temperature.

[1] e^{tA} stochastic $\Rightarrow \ker(A) = \langle \mathbb{1} \rangle$

Introducing graphs

Graph $G = (V, E)$, with

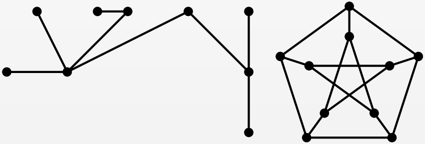
- V vertex set
- E edge set

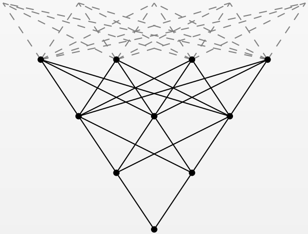


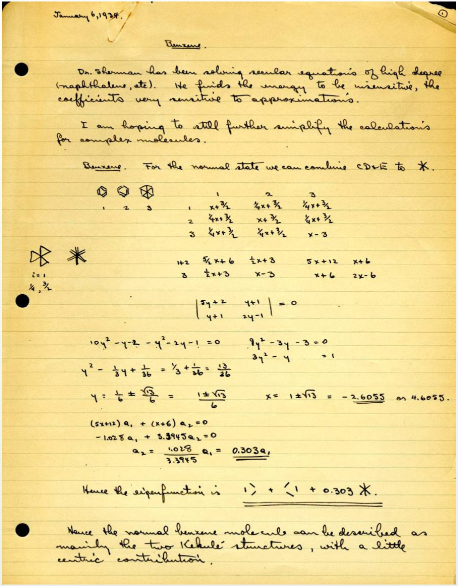
Introducing graphs

Graph $G = (V, E)$, with

- V vertex set
- E edge set







January 6, 1934.

Benzene.

Dr. Sherman has been solving secular equations of high degree (naphthalene, etc). He finds the energy to be insensitive, the coefficients very sensitive to approximations.

I am hoping to still further simplify the calculations for complex molecules.

Benzene. For the normal state we can combine CD&E to ✳.

1 2 3

	1	2	3
1	$x + 3/2$	$1/4 x + 3/2$	$1/4 x + 3/2$
2	$1/4 x + 3/2$	$x + 3/2$	$1/4 x + 3/2$
3	$1/4 x + 3/2$	$1/4 x + 3/2$	$x - 3$

$i = 1$

$1/4,\ 3/2$

1+2	$5/2 x + 6$	$\frac{1}{2} x + 3$	$5x + 12$	$x + 6$
3	$\frac{1}{2} x + 3$	$x - 3$	$x + 6$	$2x - 6$

$$\begin{vmatrix} 5y+2 & y+1 \\ y+1 & 2y-1 \end{vmatrix} = 0$$

$$10y^2 - y - 2 - y^2 - 2y - 1 = 0 \qquad 9y^2 - 3y - 3 = 0$$

$$3y^2 - y = 1$$

$$y^2 - \tfrac{1}{3}y + \tfrac{1}{36} = \tfrac{1}{3} + \tfrac{1}{36} = \tfrac{13}{36}$$

$$y = \tfrac{1}{6} \pm \tfrac{\sqrt{13}}{6} = \frac{1 \pm \sqrt{13}}{6} \qquad x = 1 \pm \sqrt{13} = -2.6055 \text{ or } 4.6055.$$

$$(5x+12)\,a_1 + (x+6)\,a_2 = 0$$

$$-1.028\,a_1 + 3.3945\,a_2 = 0$$

$$a_2 = \frac{1.028}{3.3945}\,a_1 = 0.303\,a_1$$

Hence the eigenfunction is ⟩ + ⟨ + 0.303 ✳.

Hence the normal benzene molecule can be described as mainly the two Kekulé structures, with a little centric contribution.

Description of a graph

- via the *adjacency matrix* $\mathcal{A} := (a_{\mathsf{vw}})$

$$a_{\mathsf{vw}} := \begin{cases} 1 & \text{if v is adjacent to w (``v} \sim \text{w'')} \\ 0 & \text{otherwise;} \end{cases}$$

$\operatorname{Trace} \mathcal{A} = 0 \rightsquigarrow \mathcal{A}$ has strictly positive *and* strictly negative eigenvalues.

Geršgorin's Theorem

Semyon Aronovich Geršgorin
1901–1933

Theorem (Geršgorin 1931)

All eigenvalues of a matrix $C = (c_{ij})$ are contained in

$$\bigcup_i B(c_{ii}; R_i)$$

where $R_i := \sum_{j \neq i} |c_{ij}|$.

Idea! Shift the matrix $-\mathcal{A}$ (or $+\mathcal{A}$) by $\mathcal{D} = \mathrm{diag}(\mathrm{deg}(\mathrm{v}))$ with

$$\mathrm{deg}(\mathrm{v}) := \sum_{\mathrm{w} \neq \mathrm{v}} a_{\mathrm{vw}}$$

to guarantee that all eigenvalues are ≥ 0.

Description of a graph

- via the *adjacency matrix* $\mathcal{A} := (a_{\mathsf{vw}})$

$$a_{\mathsf{vw}} := \begin{cases} 1 & \text{if v is adjacent to w (“v} \sim \text{w”)} \\ 0 & \text{otherwise;} \end{cases}$$

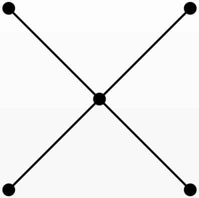
- via the *Laplacian matrix* $\mathcal{L} := \mathcal{D} - \mathcal{A}$, i.e.,

$$\mathcal{L}u_{\mathsf{v}} := \sum_{\mathsf{w} \sim \mathsf{v}} u_{\mathsf{v}} - u_{\mathsf{w}}$$

where

$$\mathcal{D} := \operatorname{diag}(\deg(\mathsf{v})_{\mathsf{v} \in \mathsf{V}}) = \operatorname{diag}(\mathcal{A}\mathbb{1})$$

Example

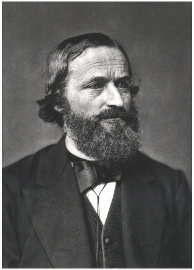


$$\mathcal{A}_G = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \mathcal{L}_G = \begin{pmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{pmatrix}$$

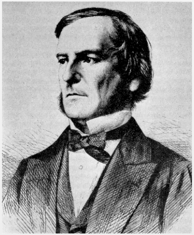
Observe: $\mathcal{A}_G, \mathcal{L}_G$ are irreducible.

More generally: $\mathcal{A}_G$ (and then $\mathcal{L}_G$, too) is irreducible iff G is connected.

Alternative description of the Laplacian, after Kirchhoff and Boole



Gustav Robert Kirchhoff
1824–1887



George Boole
1815–1864

- Assign an orientation to each edge of G: $e \equiv \overrightarrow{v\,w}$ ("e starts in v and ends in w")
- Introduce the *signed incidence matrix* $\mathcal{I} = (\iota_{ve})$:

$$\iota_{ve} := \begin{cases} +1 & \text{if e starts in v} \\ -1 & \text{if e ends in v} \\ 0 & \text{otherwise} \end{cases}$$

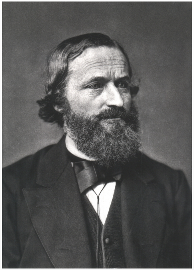
- Then $\mathcal{L} = \mathcal{I}\mathcal{I}^T$, and this does *not* depend on the chosen orientation of the edges.

Therefore: $\mathcal{L}$ is Hermitian, positive semidefinite:

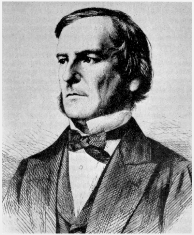
$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{\#V} \leq 2\deg_{max}$$

- $m(0) = \#$ of connected components of G
- If G is connected: $\ker(A) = \langle \mathbb{1} \rangle$ ($\rightsquigarrow P_{\ker(A)} = \frac{1}{\#V}\mathbb{1}\cdot\mathbb{1}^T$) and $m(\lambda_2) \in \{1, \ldots \#V - 1\}$

Alternative description of the Laplacian, after Kirchhoff and Boole



Gustav Robert Kirchhoff
1824–1887



George Boole
1815–1864

- Assign an orientation to each edge of G: $e \equiv \overrightarrow{v\,w}$ ("e starts in v and ends in w")
- Introduce the *signed incidence matrix* $\mathcal{I} = (\iota_{ve})$:

$$\iota_{ve} := \begin{cases} +1 & \text{if e starts in v} \\ -1 & \text{if e ends in v} \\ 0 & \text{otherwise} \end{cases}$$

- Then $\mathcal{L} = \mathcal{I}\mathcal{I}^T$, and this does *not* depend on the chosen orientation of the edges.

Therefore: $\mathcal{L}$ is Hermitian, positive semidefinite:

$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{\#V} \leq 2\,\deg_{max}$$

- $m(0) = \#$ of connected components of G
- If G is connected: $\ker(A) = \langle \mathbb{1} \rangle$ ($\rightsquigarrow P_{\ker(A)} = \frac{1}{\#V}\mathbb{1} \cdot \mathbb{1}^T$) and $m(\lambda_2) \in \{1, \ldots \#V - 1\}$

Heat semigroup on a graph

- via exponential formula:

$$e^{-t\mathcal{L}_G} = \sum_{j=0}^{\infty} \frac{(-1)^j t^j \mathcal{L}^j}{j!} = ???$$

- via spectral theorem:

$$e^{-t\mathcal{L}_G} = \sum_{k=1}^{\#V} e^{-t\lambda_k} \varphi_k \varphi_k^T = \varphi_1 \varphi_1^T + \sum_{k=2}^{\#V} e^{-t\lambda_k} \varphi_k \varphi_k^T = ???$$

<u>If G connected:</u> $-\lambda_2 < 0$ and $\varphi_1 = \frac{1}{\sqrt{\#V}} \mathbb{1}$, so

$$\| e^{-t\mathcal{L}_G} - \frac{1}{\#V} \mathbb{1} \cdot \mathbb{1}^T \| \le e^{-t\lambda_2}$$

so structure of G $\leftrightarrow$ rate of convergence to equilibrium!

Example (Heat semigroup on 4-star)

$e^{-t\mathcal{L}_G} =$

$$\begin{pmatrix} \frac{1}{5} + \frac{4}{5}e^{-5t} & -\frac{1}{5}e^{-5t} + \frac{1}{5} & -\frac{1}{5}e^{-5t} + \frac{1}{5} & -\frac{1}{5}e^{-5t} + \frac{1}{5} & -\frac{1}{5}e^{-5t} + \frac{1}{5} \\ -\frac{1}{5}e^{-5t} + \frac{1}{5} & \frac{1}{5} + \frac{3}{4}e^{-t} + \frac{1}{20}e^{-5t} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} \\ -\frac{1}{5}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & \frac{1}{5} + \frac{3}{4}e^{-t} + \frac{1}{20}e^{-5t} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} \\ -\frac{1}{5}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & \frac{1}{5} + \frac{3}{4}e^{-t} + \frac{1}{20}e^{-5t} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} \\ -\frac{1}{5}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & -\frac{1}{4}e^{-t} + \frac{1}{20}e^{-5t} + \frac{1}{5} & \frac{1}{5} + \frac{3}{4}e^{-t} + \frac{1}{20}e^{-5t} \end{pmatrix}$$

Heat semigroup on a graph

- via exponential formula:

$$e^{-t\mathcal{L}_G} = \sum_{j=0}^{\infty} \frac{(-1)^j t^j \mathcal{L}^j}{j!} = ???$$

- via spectral theorem:

$$e^{-t\mathcal{L}_G} = \sum_{k=1}^{\#V} e^{-t\lambda_k} \varphi_k \varphi_k^T = \varphi_1 \varphi_1^T + \sum_{k=2}^{\#V} e^{-t\lambda_k} \varphi_k \varphi_k^T = ???$$

<u>If G connected:</u> $-\lambda_2 < 0$ and $\varphi_1 = \frac{1}{\sqrt{\#V}} \mathbb{1}$, so

$$\| e^{-t\mathcal{L}_G} - \frac{1}{\#V} \mathbb{1} \cdot \mathbb{1}^T \| \leq e^{-t\lambda_2}$$

so structure of G $\leftrightarrow$ rate of convergence to equilibrium!

Example (Heat semigroup on 4-star)

$e^{-t\mathcal{L}_G} =$

$$\begin{pmatrix} \frac{1}{5}+\frac{4}{5}e^{-5t} & -\frac{1}{5}e^{-5t}+\frac{1}{5} & -\frac{1}{5}e^{-5t}+\frac{1}{5} & -\frac{1}{5}e^{-5t}+\frac{1}{5} & -\frac{1}{5}e^{-5t}+\frac{1}{5} \\ -\frac{1}{5}e^{-5t}+\frac{1}{5} & \frac{1}{5}+\frac{3}{4}e^{-t}+\frac{1}{20}e^{-5t} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} \\ -\frac{1}{5}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & \frac{1}{5}+\frac{3}{4}e^{-t}+\frac{1}{20}e^{-5t} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} \\ -\frac{1}{5}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & \frac{1}{5}+\frac{3}{4}e^{-t}+\frac{1}{20}e^{-5t} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} \\ -\frac{1}{5}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & -\frac{1}{4}e^{-t}+\frac{1}{20}e^{-5t}+\frac{1}{5} & \frac{1}{5}+\frac{3}{4}e^{-t}+\frac{1}{20}e^{-5t} \end{pmatrix}$$

Heat semigroup on a graph

- via exponential formula:

$$e^{-t\mathcal{L}_G} = \sum_{j=0}^{\infty} \frac{(-1)^j t^j \mathcal{L}^j}{j!} = ???$$

- via spectral theorem:

$$e^{-t\mathcal{L}_G} = \sum_{k=1}^{\#V} e^{-t\lambda_k} \varphi_k \varphi_k^T$$

$$= \varphi_1 \varphi_1^T + \sum_{k=2}^{\#V} e^{-t\lambda_k} \varphi_k \varphi_k^T = ???$$

<u>If G connected:</u> $-\lambda_2 < 0$ and $\varphi_1 = \frac{1}{\sqrt{\#V}} \mathbb{1}$, so

$$\| e^{-t\mathcal{L}_G} - \frac{1}{\#V} \mathbb{1} \cdot \mathbb{1}^T \| \leq e^{-t\lambda_2}$$

so structure of G $\leftrightarrow$ rate of convergence to equilibrium!

Example (Heat semigroup on 4-star)

$e^{-t\mathcal{L}_G} =$

$$\begin{pmatrix}
\frac{1}{5} + \frac{4}{5} e^{-5t} & -\frac{1}{5} e^{-5t} + \frac{1}{5} & -\frac{1}{5} e^{-5t} + \frac{1}{5} & -\frac{1}{5} e^{-5t} + \frac{1}{5} & -\frac{1}{5} e^{-5t} + \frac{1}{5} \\
-\frac{1}{5} e^{-5t} + \frac{1}{5} & \frac{1}{5} + \frac{3}{4} e^{-t} + \frac{1}{20} e^{-5t} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} \\
-\frac{1}{5} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & \frac{1}{5} + \frac{3}{4} e^{-t} + \frac{1}{20} e^{-5t} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} \\
-\frac{1}{5} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & \frac{1}{5} + \frac{3}{4} e^{-t} + \frac{1}{20} e^{-5t} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} \\
-\frac{1}{5} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & -\frac{1}{4} e^{-t} + \frac{1}{20} e^{-5t} + \frac{1}{5} & \frac{1}{5} + \frac{3}{4} e^{-t} + \frac{1}{20} e^{-5t}
\end{pmatrix}$$

Graph Laplacian as generator of a Markov semigroup

Arne Beurling

1905–1986

Jacques Deny

1916–2016

Theorem (Beurling–Deny 1959)

Let G be a (finite) graph. $-\mathcal{L}_G$ generates a semigroup that is

- *positive:* $e^{-t\mathcal{L}_G} f \geq 0$ *if* $f \geq 0$;
- ℓ^∞*-contractive:* $\|e^{-t\mathcal{L}_G} f\|_\infty \leq \|f\|_\infty$;
- *stochastic:* $\|e^{-t\mathcal{L}_G} f\|_1 = \|f\|_1$ *if* $f \geq 0$, *i.e.,* $\mathbb{1}$ *is the density of an invariant measure;*
- *irreducible:* $e^{-t\mathcal{L}_G} f > 0$ *if* $f \gneq 0$ *(if G is connected).*

Proof.

- $\mathcal{L}_G$ is an *M-matrix*: $\mathcal{L}_{vv} \in \mathbb{R}$, $\mathcal{L}_{vw} \leq 0$
- $\deg(v) \geq \sum_{w \sim v} \mathcal{L}_{vw}$
- $\mathcal{L}_G \mathbb{1} = 0$, hence $e^{-t\mathcal{L}_G}\mathbb{1} \equiv \mathbb{1}$
- G connected $\Leftrightarrow$ $\mathcal{L}_G$ irreducible $\Leftrightarrow$ $e^{-t\mathcal{L}_G}$ irreducible

□

Graph Laplacian as generator of a Markov semigroup

Arne Beurling
1905–1986

Jacques Deny
1916–2016

Theorem (Beurling–Deny 1959)

Let G be a (finite) graph. $-\mathcal{L}_{\mathsf{G}}$ *generates a semigroup that is*

- *positive:* $\mathrm{e}^{-t\mathcal{L}_{\mathsf{G}}} f \geq 0$ *if* $f \geq 0$;
- ℓ^∞*-contractive:* $\|\mathrm{e}^{-t\mathcal{L}_{\mathsf{G}}} f\|_\infty \leq \|f\|_\infty$;
- *stochastic:* $\|\mathrm{e}^{-t\mathcal{L}_{\mathsf{G}}} f\|_1 = \|f\|_1$ *if* $f \geq 0$, *i.e.,* $\mathbb{1}$ *is the density of an invariant measure;*
- *irreducible:* $\mathrm{e}^{-t\mathcal{L}_{\mathsf{G}}} f > 0$ *if* $f \gneq 0$ *(if G is connected).*

Proof.

- $\mathcal{L}_{\mathsf{G}}$ is an *M-matrix*: $\mathcal{L}_{\mathsf{vv}} \in \mathbb{R}$, $\mathcal{L}_{\mathsf{vw}} \leq 0$
- $\deg(\mathsf{v}) \geq \sum_{\mathsf{w}\sim\mathsf{v}} \mathcal{L}_{\mathsf{vw}}$
- $\mathcal{L}_{\mathsf{G}}\mathbb{1} = 0$, hence $\mathrm{e}^{-t\mathcal{L}_{\mathsf{G}}}\mathbb{1} \equiv \mathbb{1}$
- G connected $\Leftrightarrow$ $\mathcal{L}_{\mathsf{G}}$ irreducible $\Leftrightarrow$ $\mathrm{e}^{-t\mathcal{L}_{\mathsf{G}}}$ irreducible

$\square$

Extension #1: Magnetic potentials

In mathematical physics:

$$\Delta \quad \rightsquigarrow \quad (\nabla + i\alpha)^2$$

magnetic potential

For $\tau \in [0, 2\pi)$, consider the *magnetic incidence matrix* $\mathcal{I}^{(\tau)} = (\iota_{\mathsf{ve}}^{(\tau)})$

$$\iota_{\mathsf{ve}}^{(\tau)} := \begin{cases} 1 & \text{if } \mathsf{e} = \overrightarrow{\mathsf{vw}} \text{ starts in } \mathsf{v} \\ \mathrm{e}^{i\tau} & \text{if } \mathsf{e} = \overrightarrow{\mathsf{vw}} \text{ ends in } \mathsf{v} \\ 0 & \text{otherwise} \end{cases}$$

and the **magnetic Laplacian** $\mathcal{L}_\tau := \mathcal{I}_\tau \mathcal{I}_\tau^T$.

- $\mathcal{L}_{\mathsf{G}} = \mathcal{L}_{-\pi}$;
- $\mathcal{L}_{\mathsf{G}}$ is the *comparison matrix* of $\mathcal{L}_\tau$, for all τ;
- $\mathrm{e}^{-t\mathcal{L}_{\mathsf{G}}} = \mathrm{e}^{-t\mathcal{L}_{-\pi}}$ is the *modulus semigroup* of $\mathrm{e}^{-t\mathcal{L}_{-\tau}}$, for all τ.

Extension #2: Failure of Markov property

Consider the **bi-Laplacian** $\mathcal{L}^2_{\mathsf{G}}$:

- $e^{t\mathcal{L}^2}$ is a contractive semigroup on $\ell^2(\mathsf{V})$;
- (Gregorio–M. 2021) TFAE:
  - $e^{t\mathcal{L}^2_{\mathsf{G}}}$ is positive;
  - $e^{t\mathcal{L}^2_{\mathsf{G}}}$ is ℓ^∞-contractive;
  - G is the complete graph.

Proposition (Gregorio–M. 2021)

$e^{t\mathcal{L}^2_{\mathsf{G}}}$ is <u>for all connected G</u> eventually Markovian and irreducible, i.e., for some $t_0 = t_0(\mathsf{G}) > 0$ and all $t \geq t_0$

- $e^{t\mathcal{L}^2_{\mathsf{G}}} f > 0$ *for all* $f \gneq 0$;
- $\|e^{t\mathcal{L}^2_{\mathsf{G}}} f\|_\infty \leq \|f\|_\infty$.

Extension #2: Failure of Markov property

Consider the **bi-Laplacian** $\mathcal{L}^2_{\mathsf{G}}$:

- $e^{t\mathcal{L}^2}$ is a contractive semigroup on $\ell^2(\mathsf{V})$;
- (Gregorio–M. 2021) TFAE:
  - $e^{t\mathcal{L}^2_{\mathsf{G}}}$ is positive;
  - $e^{t\mathcal{L}^2_{\mathsf{G}}}$ is ℓ^∞-contractive;
  - G is the complete graph.

Proposition (Gregorio–M. 2021)

$e^{t\mathcal{L}^2_{\mathsf{G}}}$ *is for all connected* G *eventually Markovian and irreducible, i.e., for some* $t_0 = t_0(\mathsf{G}) > 0$ *and all* $t \geq t_0$

- $e^{t\mathcal{L}^2_{\mathsf{G}}} f > 0$ *for all* $f \gneq 0$;
- $\|e^{t\mathcal{L}^2_{\mathsf{G}}} f\|_\infty \leq \|f\|_\infty$.

Extensions #3: Flows in space of probabilities

Theorem (Erbar–Maas 2014)

The heat flow in $\mathcal{G} = (\mathsf{V}, \mathsf{E})$ *can be studied as a flow of a functional in a space of probabilities over* V.

Proof.

Discrete Benamou–Brenier-type formula (Maas 2011).´ □

C_0-semigroups

Definition

*Let E be a normed space. A C_0-**semigroup** is a family $(T(t))_{t\geq 0}$ of bounded linear operators on E such that*

- $T(0) = \mathrm{Id}$
- $T(t+s) = T(t)T(s)$
- $\lim_{t\to 0} T(t)f = f$ *for all* $f \in E$.

Example

$T(t)f(\cdot) = f(t+\cdot)$ is a C_0 semigroup on $E = L^p(\mathbb{R})$ for any $p \in [1,\infty)$.
(But not for $p = \infty$: Exercise.)

Example

$T(t)f(\cdot) = \mathrm{e}^{tq(\cdot)}f(\cdot)$ is a C_0 semigroup on $E = L^p(\Omega)$ for any $p \in [1,\infty)$ and any $q \in L^\infty(X)$.

Generators

Definition

An operator A on E is a **generator** *of a C_0-semigroup $(T(t))_{t\geq 0}$ on E if*

$$D(A) = \left\{ f \in E : \exists \lim_{t \geq 0+} \frac{T(t)f - f}{t} \right\}$$

$$Af = \lim_{t \to 0+} \frac{T(t)f - f}{t}.$$

Example

$T(t)f(\cdot) = f(t + \cdot)$ on $L^p(\mathbb{R})$ is generated by

$$D(A) = W^{1,p}(\mathbb{R})$$

$$Af = f'.$$

Example

$T(t)f(\cdot) = \mathrm{e}^{tq(\cdot)} f(\cdot)$ on $L^p(\Omega)$, $\Omega \subset \mathbb{R}^d$ is generated by

$$D(A) = L^p(\Omega)$$

$$Af = qf.$$

Proposition

For a generator A of a C_0-semigroup $(T(t))_{t\geq 0}$ on E the following hold:

- *A is linear;*
- *if $f \in D(A)$, then $T(t)f \in D(A)$ and $\frac{\mathrm{d}}{\mathrm{d}t}T(t)f = T(t)Af = AT(t)f$ for all $t \geq 0$;*
- *A is closed and densely defined;*
- *$(T(t))_{t\geq 0}$ determines its generator uniquely, and vice versa;*
- $\mathrm{Ker}(A) = \{f \in E : T(t)f = f \ \forall t \geq 0\}$.

Proof.

Exercise □

The C_0-semigroup generated by A is denoted by $(\mathrm{e}^{tA})_{t\geq 0}$.

Analytic semigroups

Definition

A C_0-semigroup $(\mathrm{e}^{tA})_{t\geq 0}$ is **analytic** *if*

$$\|tA\mathrm{e}^{tA}f\| \leq c\|f\|$$

for some $c > 0$ and all $t \in (0,1]$ and $f \in D(A)$.

In particular,

$$\|A\mathrm{e}^{tA}f\| \leq c(t)\|f\|$$

i.e., e^{tA} is bounded from E to $D(A)$, hence (Exercise) from E to $\bigcap_{k\in\mathbb{N}} D(A^k)$, for all $t > 0$.

Example

- $T(t)f(\cdot) = \mathrm{e}^{tq(\cdot)}f(\cdot)$ is analytic, for any $q \in L^\infty(\Omega)$;
- $T(t)f(\cdot) = f(t + \cdot)$ is NOT analytic.

Remark

A C_0-semigroup $(\mathrm{e}^{t\Delta_\mathcal{G}})_{t\geq 0}$ is analytic if and only if for some $\theta \in (0, \pi)$ it has an analytic extension $(\mathrm{e}^{t\Delta_\mathcal{G}})_{t\in\Sigma_\theta}$ that is bounded on $\Sigma_\theta \cap \{z \in \mathbb{C} : |z| \leq 1\}$, where

$$\Sigma_\theta := \{r\mathrm{e}^{i\alpha} : r > 0,\ |\alpha| < \theta\}.$$

Theorem (Bifulco–M. 2025)

If A generates on $E = L^2(\Omega;\mu)$ an analytic semigroup, and if $D(A^k), D(A'^k) \hookrightarrow C_b(\Omega)$, then there is a pointwise heat kernel associated with A and

$$T(t)f = \int_X p_t(\cdot, y) f(y)\,\mathrm{d}\mu(y), \qquad t \geq 0.$$

Heat kernels

(Ω, d, μ) metric measure space, A operator on $L^p(\Omega; \mu)$

$p = p_t(x, y) : (0, \infty) \times \Omega \times \Omega \to \mathbb{C}$ is a **heat kernel** associated with A

1. $p_t(\cdot, \cdot) : X \times X \to \mathbb{C}$ is measurable; $p_t(x, \cdot) \in L^{p'}(X)$ and $p_t(x, \cdot)f(\cdot) \in L^1(X)$, for all $f \in L^p(X)$, $t > 0$, a.e. $x \in \Omega$;
2. $x \mapsto \int_\Omega p_t(x, y)f(y)\,\mathrm{d}\mu(y)$ belongs to $L^p(\Omega)$ for all $t > 0$, $f \in L^p(\Omega)$;
3. $p_{t+s}(x, y) = \int_\Omega p_t(x, z)p_s(z, y)\,\mathrm{d}\mu(z)$ for all $s, t > 0$, a.e. $(x, y) \in \Omega \times \Omega$;
4. $t \mapsto p_t(\cdot, y)$ belongs to $C^1\left((0, \infty); L^p(\Omega)\right) \cap C\left((0, \infty); D(A_x)\right)$ for a.e. $y \in \Omega$,
5. $\frac{\partial}{\partial t} p_t(\cdot, y) = A_x p_t(\cdot, y)$ for all $t > 0$, a.e. $y \in \Omega$.
6. $\lim_{t \to 0^+} \int_X p_t(\cdot, y)f(y)\,\mathrm{d}\mu(y) = f(\cdot)$ (in $L^p(\Omega)$) for all $f \in L^p(\Omega)$

pointwise heat kernel if (i), (iii), (iv), (v) hold for all $x, y \in \Omega$.

Let A be differential operator on $L^2(\Omega)$ (with BC)

- If there is a heat kernel associated with A, then

$$(*) \qquad \begin{cases} \dfrac{\partial u}{\partial t}(t,x) = Au(t,x) & t \geq 0,\ x \in \Omega \\ u(0,x) = u_0(x) & x \in \Omega \end{cases}$$

  is well-posed: i.e.,
  - for each u_0 there is a solution of $(*)$;
  - such a solution is unique;
  - the solution continuously depends on u_0.

- But: $(*)$ well-posed $\not\Rightarrow$ A has a heat kernel:
  e.g. $\Omega = \mathbb{R}$, $A = \frac{\partial}{\partial x} \rightsquigarrow u(t,x) = \int_{\mathbb{R}} \delta_{x+t}(y) u_0(y)\,\mathrm{d}y$
  but $p_t(\cdot, y) = \delta_{\cdot+t}(y) \in H^{-1}(\mathbb{R}) \setminus L^\infty(\mathbb{R})\ \forall y$.

- A has a heat kernel $\not\Rightarrow$

$$p_t(x,y) = \sum_{k \in \mathbb{N}} \mathrm{e}^{-t\lambda_k} \varphi_k(x)\varphi_k(y)$$

  e.g. $\Omega = \mathbb{R}$, $A = \frac{\partial^2}{\partial x^2}$, $p_t(x,y) = \frac{1}{\sqrt{4\pi t}} \mathrm{e}^{-\frac{|x-y|^2}{4t}}$ but no eigenvalues
  (or for Schrödinger operators: embedded eigenvalues may exist)

Let A be differential operator on $L^2(\Omega)$ (with BC)

- If there is a heat kernel associated with A, then

$$(*) \qquad \begin{cases} \dfrac{\partial u}{\partial t}(t,x) = Au(t,x) & t \geq 0,\ x \in \Omega \\ u(0,x) = u_0(x) & x \in \Omega \end{cases}$$

  is well-posed: i.e.,
  - for each u_0 there is a solution of $(*)$;
  - such a solution is unique;
  - the solution continuously depends on u_0.
- But: $(*)$ well-posed $\not\Rightarrow$ A has a heat kernel:
  e.g. $\Omega = \mathbb{R}$, $A = \frac{\partial}{\partial x}$ $\rightsquigarrow$ $u(t,x) = \int_{\mathbb{R}} \delta_{x+t}(y) u_0(y)\,\mathrm{d}y$
  but $p_t(\cdot, y) = \delta_{\cdot+t}(y) \in H^{-1}(\mathbb{R}) \setminus L^\infty(\mathbb{R})\ \forall y$.
- A has a heat kernel $\not\Rightarrow$

$$p_t(x,y) = \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} \varphi_k(x)\varphi_k(y)$$

  e.g. $\Omega = \mathbb{R}$, $A = \frac{\partial^2}{\partial x^2}$, $p_t(x,y) = \frac{1}{\sqrt{4\pi t}} \mathrm{e}^{-\frac{|x-y|^2}{4t}}$ but no eigenvalues
  (or for Schrödinger operators: embedded eigenvalues may exist)

Let A be differential operator on $L^2(\Omega)$ (with BC)

- If there is a heat kernel associated with A, then

$$(*)\qquad \begin{cases} \dfrac{\partial u}{\partial t}(t,x) = Au(t,x) & t \geq 0,\ x \in \Omega \\ u(0,x) = u_0(x) & x \in \Omega \end{cases}$$

  is well-posed: i.e.,
    - for each u_0 there is a solution of $(*)$;
    - such a solution is unique;
    - the solution continuously depends on u_0.
- But: $(*)$ well-posed $\not\Rightarrow$ A has a heat kernel:
  e.g. $\Omega = \mathbb{R}$, $A = \frac{\partial}{\partial x} \rightsquigarrow u(t,x) = \int_{\mathbb{R}} \delta_{x+t}(y) u_0(y)\,\mathrm{d}y$
  but $p_t(\cdot, y) = \delta_{\cdot+t}(y) \in H^{-1}(\mathbb{R}) \setminus L^\infty(\mathbb{R})\ \forall y$.
- A has a heat kernel $\not\Rightarrow$

$$p_t(x,y) = \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} \varphi_k(x)\varphi_k(y)$$

  e.g. $\Omega = \mathbb{R}$, $A = \frac{\partial^2}{\partial x^2}$, $p_t(x,y) = \frac{1}{\sqrt{4\pi t}} \mathrm{e}^{-\frac{|x-y|^2}{4t}}$ but no eigenvalues
  (or for Schrödinger operators: embedded eigenvalues may exist)

$$p_t(x,y) = \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k}\varphi_k(x)\varphi_k(y),$$

- useful for numerical purposes (stay tuned)
- difficult to use to deduce qualitative properties of the heat equation.

Prototypical Example (Heat equation on $(0,\ell)$ with Dirichlet conditions)

$\Omega = (0,\ell)$: $A = \frac{\partial^2}{\partial x^2}$ *with* $D(A) := H^2(0,\ell)\cap H^1_0(0,\ell)$.

$$p_t(x,y) = \frac{2}{\ell}\sum_{k=1}^{\infty} \mathrm{e}^{-t\frac{\pi^2k^2}{\ell^2}} \sin\left(\frac{\pi k x}{\ell}\right)\sin\left(\frac{\pi k y}{\ell}\right)$$

$$p_t(x,x) = \frac{2}{\ell}\sum_{k=1}^{\infty} \mathrm{e}^{-t\frac{\pi^2k^2}{\ell^2}} \sin^2\left(\frac{\pi k x}{\ell}\right) \geq \frac{2}{\ell}\mathrm{e}^{-t\frac{\pi^2}{\ell^2}} \sin^2\left(\frac{\pi x}{\ell}\right) \overset{t\approx 0}{\approx} \frac{2}{\ell}\sin^2\left(\frac{\pi x}{\ell}\right) \overset{x=\frac{\ell}{2}}{=} \frac{2}{\ell}$$

So, p_t need not be ≤ 1 pointwise unless Ω is an atomic measure space.

$$p_t(x,y) = \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k}\varphi_k(x)\varphi_k(y),$$

- useful for numerical purposes (stay tuned)
- difficult to use to deduce qualitative properties of the heat equation.

Prototypical Example (Heat equation on $(0,\ell)$ with Dirichlet conditions)

$\Omega = (0,\ell)$: $A = \frac{\partial^2}{\partial x^2}$ *with* $D(A) := H^2(0,\ell)\cap H^1_0(0,\ell)$.

$$p_t(x,y) = \frac{2}{\ell}\sum_{k=1}^{\infty} \mathrm{e}^{-t\frac{\pi^2 k^2}{\ell^2}} \sin(\frac{\pi k x}{\ell})\sin(\frac{\pi k y}{\ell})$$

$$p_t(x,x) = \frac{2}{\ell}\sum_{k=1}^{\infty} \mathrm{e}^{-t\frac{\pi^2 k^2}{\ell^2}} \sin^2(\frac{\pi k x}{\ell}) \geq \frac{2}{\ell}\mathrm{e}^{-t\frac{\pi^2}{\ell^2}}\sin^2(\frac{\pi x}{\ell}) \overset{t\approx 0}{\approx} \frac{2}{\ell}\sin^2(\frac{\pi x}{\ell}) \overset{x=\frac{\ell}{2}}{=} \frac{2}{\ell}$$

So, p_t need not be ≤ 1 pointwise unless Ω is an atomic measure space.

$$p_t(x,y) = \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k}\varphi_k(x)\varphi_k(y),$$

- useful for numerical purposes (stay tuned)
- difficult to use to deduce qualitative properties of the heat equation.

Prototypical Example (Heat equation on $(0,\ell)$ with Dirichlet conditions)

$\Omega = (0,\ell)$: $A = \frac{\partial^2}{\partial x^2}$ *with* $D(A) := H^2(0,\ell)\cap H^1_0(0,\ell)$.

$$p_t(x,y) = \frac{2}{\ell}\sum_{k=1}^{\infty} \mathrm{e}^{-t\frac{\pi^2k^2}{\ell^2}} \sin(\frac{\pi kx}{\ell})\sin(\frac{\pi ky}{\ell})$$

$$p_t(x,x) = \frac{2}{\ell}\sum_{k=1}^{\infty} \mathrm{e}^{-t\frac{\pi^2k^2}{\ell^2}} \sin^2(\frac{\pi kx}{\ell}) \geq \frac{2}{\ell}\mathrm{e}^{-t\frac{\pi^2}{\ell^2}} \sin^2(\frac{\pi x}{\ell}) \overset{t\approx 0}{\approx} \frac{2}{\ell}\sin^2(\frac{\pi x}{\ell}) \overset{x=\frac{\ell}{2}}{=} \frac{2}{\ell}$$

So, p_t need not be ≤ 1 pointwise unless Ω is an atomic measure space.

$$p_t(x,y) = \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k}\varphi_k(x)\varphi_k(y),$$

- useful for numerical purposes (stay tuned)
- difficult to use to deduce qualitative properties of the heat equation.

Prototypical Example (Heat equation on $(0,\ell)$ with Dirichlet conditions)

$\Omega = (0,\ell)$: $A = \frac{\partial^2}{\partial x^2}$ *with* $D(A) := H^2(0,\ell)\cap H^1_0(0,\ell)$.

$$p_t(x,y) = \frac{2}{\ell}\sum_{k=1}^{\infty} \mathrm{e}^{-t\frac{\pi^2k^2}{\ell^2}} \sin(\frac{\pi kx}{\ell})\sin(\frac{\pi ky}{\ell})$$

$$p_t(x,x) = \frac{2}{\ell}\sum_{k=1}^{\infty} \mathrm{e}^{-t\frac{\pi^2k^2}{\ell^2}} \sin^2(\frac{\pi kx}{\ell}) \geq \frac{2}{\ell}\mathrm{e}^{-t\frac{\pi^2}{\ell^2}}\sin^2(\frac{\pi x}{\ell}) \overset{t\approx 0}{\approx} \frac{2}{\ell}\sin^2(\frac{\pi x}{\ell}) \overset{x=\frac{\ell}{2}}{=} \frac{2}{\ell}$$

So, p_t need not be ≤ 1 pointwise unless Ω is an atomic measure space.

How to recover qualitative properties?

- $p_t(\cdot,\cdot) > 0 \ \forall t \Leftrightarrow$ parabolic strong maximum principle
  (i.e., $u_0 \geq 0,\ u \not\equiv 0 \Rightarrow u(t,\cdot) > 0 \ \forall t$)
- $0 \leq p_t(\cdot,\cdot)$ and $\int p_t(x,y)\,\mathrm{d}y = 1 \ \forall t, x \Leftrightarrow$ Markov property
  (i.e., $0 \leq u_0 \leq 1 \Rightarrow 0 \leq u(t,\cdot) \leq 1 \ \forall t$)
- $\|p_t(\cdot,\cdot)\|_{L^1} \equiv |\Omega| \ \forall t \Leftrightarrow$ stochastic
  (i.e., $0 \leq u_0 \Rightarrow \|u(t,\cdot)\|_{L^1} = \|u_0\|_{L^1} \ \forall t$)
- $|p_t^{(1)}(x,y)| \leq p_t^{(2)}(x,y) \Leftrightarrow$ domination
  (i.e., $|u_0^{(1)}| \leq u_0^{(2)} \Rightarrow |u^{(1)}(t)| \leq u^{(2)}(t) \ \forall t$)
- $p_t(\cdot,\cdot) \in C^\infty(\Omega \times \Omega) \ \forall t > 0 \Leftrightarrow$ smoothing effect
  (i.e., $u_0 \in \mathcal{D}'(\Omega) \Rightarrow u(t,\cdot) \in C^\infty(\Omega) \ \forall t$); Schwartz–Hörmander

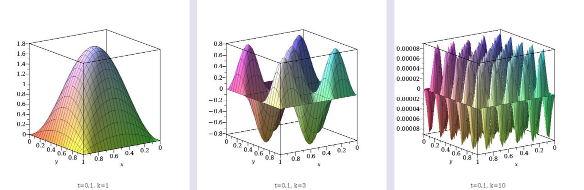
Prototypical Example (Heat equation on $(0,1)$ with Dirichlet conditions)

$\Omega = (0,1)$: $A = \frac{\partial^2}{\partial x^2}$ *with* $D(A) := H^2(0,1) \cap H_0^1(0,1)$.
Then $\lambda_k = k^2\pi^2$, $\phi_k(x) = \sqrt{2}\sin(\pi k x)$, $k \in \mathbb{N}$. *and*

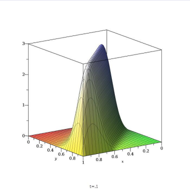
$$p_t(x,y) = 2\sum_{k=1}^{\infty} \mathrm{e}^{-t\pi^2 k^2} \sin(\pi k x)\sin(\pi k y)$$

$p_t(x,y) \geq 0$: **Is this true?**

addends of the heat kernel:



heat kernel:



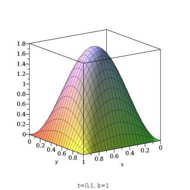
Prototypical Example (Heat equation on $(0,1)$ with Dirichlet conditions)

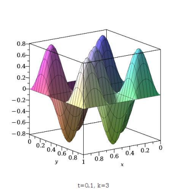
$\Omega = (0,1)$: $A = \frac{\partial^2}{\partial x^2}$ *with* $D(A) := H^2(0,1) \cap H_0^1(0,1)$.
Then $\lambda_k = k^2\pi^2$, $\phi_k(x) = \sqrt{2}\sin(\pi k x)$, $k \in \mathbb{N}$. *and*

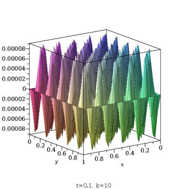
$$p_t(x,y) = 2\sum_{k=1}^{\infty} \mathrm{e}^{-t\pi^2 k^2} \sin(\pi k x)\sin(\pi k y)$$

$p_t(x,y) \geq 0$: **Is this true?**

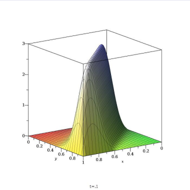
addends of the heat kernel:



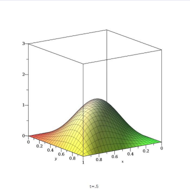




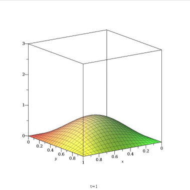
heat kernel:



$\rightarrow$



$\rightarrow$



A workaround: quadratic forms

Any closed quadratic form $\mathfrak{A}$ on $L^2(\Omega;\mu)$ is associated with a unique self-adjoint, positive semi-definite operator A on $L^2(\Omega;\mu)$, and vice versa: there holds

$$D(A) = \{f \in D(\mathfrak{A}) : \exists g \in L^2(\Omega;\mu) \text{s.t. } \mathfrak{a}(f,h) = \langle g,h\rangle \ \forall h \in D(\mathfrak{A})\}$$
$$Af = -g$$

where $\mathfrak{a}$ is the bilinear form corresponding with $\mathfrak{A}$, i.e.,

$$\mathfrak{A}(f) = \frac{1}{2}\mathfrak{a}(f,f) \qquad f \in D(\mathfrak{a}) = D(\mathfrak{A}).$$

Furthermore, A has compact resolvent iff $D(\mathfrak{A})$ is compactly embedded in $L^2(\Omega;\mu)$.

Remark

Equivalently: $A = -\partial_{L^2}\mathfrak{A}$ (Exercise). But: Associated operators on L^2 can be defined even for non-symmetric forms! Idea: use Lax–Milgram instead of Riesz–Fréchet.

Self-adjoint operators and the Spectral Theorem

Let A be a self-adjoint, negative semidefinite operator on $L^2(\Omega;\mu)$ with compact resolvent.
Then

- $L^2(\Omega;\mu)$ has an ONB of eigenvectors of A: $(\varphi_k)_{k\in\mathbb{N}} \sim (-\lambda_k)_{k\in\mathbb{N}}$;
- A can be diagonalized:

$$D(A) = \left\{ f \in L^2(\Omega;\mu) : \sum_{k\in\mathbb{N}} \lambda_k^2 \langle f, \varphi_k\rangle^2 < \infty \right\},$$

$$Af = -\sum_{k\in\mathbb{N}} \lambda_k \langle f, \varphi_k\rangle \varphi_k$$

- A is associated with a closed quadratic form $\mathfrak{A} \simeq \mathfrak{a}$ given by

$$D(\mathfrak{a}) = \left\{ f \in L^2(\Omega;\mu) : \sum_{k\in\mathbb{N}} \lambda_k \langle f, \varphi_k\rangle^2 < \infty \right\}$$

$$\mathfrak{a}(f,g) = \sum_{k\in\mathbb{N}} \lambda_k \langle f, \varphi_k\rangle \langle \varphi_k, g\rangle.$$

! $\lambda_k \geq 0$

Semigroups associatd with closed quadratic forms

Proposition

Every self-adjoint, negative semidefinite operator generates an analytic semigroup.

Proof.

For simplicity, only for operators with compact resolvent:

- By functional calculus, $\mathrm{e}^{tA} := \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k}\langle f, \varphi_k\rangle\varphi_k$ is a well-defined bounded linear operator on $L^2(\Omega;\mu)$;
- Given $f \in D(A)$ and $t > 0$

$$\|tA\mathrm{e}^{tA}f\|^2 = \|t\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{tA}f\|^2 = \sum_{k\in\mathbb{N}} |t\lambda_k \mathrm{e}^{-t\lambda_k}\langle f, \varphi_k\rangle|^2 \leq \frac{1}{\mathrm{e}}\|f\|^2$$

□

Qualitative properties vs invariance properties via semigroups

El Maati Ouhabaz

1965–

Theorem (Ouhabaz 1996)

Let $(\Omega;\mu)$ be a measure space. Let $\mathfrak{A}$ be a quadratic form associated with a semigroup e^{tA} on $L^2(\Omega)$. Let C be a closed convex set of $L^2(\Omega)$. TFAE:

- $\mathrm{e}^{tA}C \subset C$ for all $t \geq 0$.
- $u \in D(\mathfrak{A})$ and $\mathfrak{a}(P_C u) \leq \mathfrak{a}(u)$ for all $u \in D(\mathfrak{A})$.
- $u \in D(\mathfrak{A})$ and $\mathrm{Re}\,\mathfrak{a}(P_C u, u - P_C u) \geq 0$ for all $u \in D(\mathfrak{A})$.

Corollary (Beurling–Deny 1959)

e^{tA} is positive iff $u^+ \in D(\mathfrak{A})$ and $\mathfrak{A}(u^+) \leq \mathfrak{A}(u)$ for all $u \in D(\mathfrak{A})$.

Introducing metric graphs

Figure: Valentina Vetturi, *Tails*, 2023

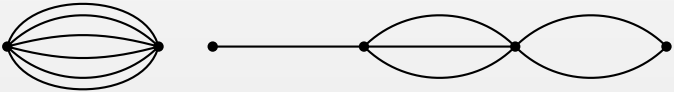
Introducing metric graphs

Let

- $E = \{e_1, e_2, \dots\}$ <u>finite</u> set ("edge set")
- $\ell : E \to (0, \infty]$ ("edge lengths")
- a metric measure structure (d_e, μ_e) on each edge $[0, \ell_e]$
- $\sim$ equivalence relation on $\mathcal{V} := \bigsqcup_{e \in E} \{0, \ell_e\}$ ("wiring")

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

Then $\mathcal{G} := \mathcal{E}/\sim$ is a **metric graph** and $V := \mathcal{V}/\sim$ its **vertex set**.



$G := (V, E)$ is the **underlying combinatorial graph** of $\mathcal{G}$.

$\mathcal{G}$ inherits a

- metric d (shortest path metric induced by $(d_e)_{e \in E}$)
- measure μ (direct sum of $(\mu_e)_{e \in E}$)

structure from the MMS structure on each edge.

- Topological features (number κ of connected components, Betti number $\beta := \#E - \#V + \kappa$, etc.) are determined by $\sim$;
- metric features (diameter) by d;
- measure features (finite measure) by μ.

Unless otherwise mentioned, for all $e \in E$:

- $\ell_e < \infty$;
- $d_e \equiv$ Euclidean distance
- $\mu_e \equiv$ Lebesgue measure

In this case: $\mathcal{G}$ is a compact metric space of finite measure.

Goal: define a Laplacian on $\mathcal{G}$ by means of a quadratic function on $L^2(\mathcal{G})$.
Idea: integrate $-\Delta_{\mathcal{G}} f \in L^2(\mathcal{G})$ against a test function $h \in C(\mathcal{G}) \cap L^2(\mathcal{G})$.

$$\begin{aligned}
(-\Delta_{\mathcal{G}} f, h) &= \int_{\mathcal{G}} f''(x)h(x)\,\mathrm{d}x \\
&= -\sum_{\mathsf{e}\in\mathsf{E}} \int_0^{\ell_\mathsf{e}} f_\mathsf{e}''(x)h_\mathsf{e}(x)\,\mathrm{d}x \\
&= -\sum_{\mathsf{e}\in\mathsf{E}} f_\mathsf{e}'(x)h_\mathsf{e}(x)\,\mathrm{d}x\Big|_{x=0}^{x=\ell_\mathsf{e}} + \sum_{\mathsf{e}\in\mathsf{E}} \int_0^{\ell_\mathsf{e}} f_\mathsf{e}'(x)h_\mathsf{e}'(x)\,\mathrm{d}x \\
&\overset{!}{=} -h(\mathsf{v})\sum_{\mathsf{e}\sim\mathsf{v}} \frac{\partial f_\mathsf{e}}{\partial n}(\mathsf{v}) + \sum_{\mathsf{e}\in\mathsf{E}} \int_0^{\ell_\mathsf{e}} f_\mathsf{e}'(x)h_\mathsf{e}'(x)\,\mathrm{d}x \\
&\overset{?}{=} \sum_{\mathsf{e}\in\mathsf{E}} \int_0^{\ell_\mathsf{e}} f_\mathsf{e}'(x)h_\mathsf{e}'(x)\,\mathrm{d}x = \mathfrak{a}(f,h)
\end{aligned}$$

Goal: define a Laplacian on $\mathcal{G}$ by means of a quadratic function on $L^2(\mathcal{G})$.
Idea: integrate $-\Delta_{\mathcal{G}} f \in L^2(\mathcal{G})$ against a test function $h \in C(\mathcal{G}) \cap L^2(\mathcal{G})$.

$$\begin{aligned}
(-\Delta_{\mathcal{G}} f, h) &= -\int_{\mathcal{G}} f''(x) h(x)\,\mathrm{d}x \\
&= -\sum_{\mathsf{e}\in\mathsf{E}} \int_0^{\ell_\mathsf{e}} f_\mathsf{e}''(x) h_\mathsf{e}(x)\,\mathrm{d}x \\
&= -\sum_{\mathsf{e}\in\mathsf{E}} f_\mathsf{e}'(x) h_\mathsf{e}(x)\,\mathrm{d}x \Big|_{x=0}^{x=\ell_\mathsf{e}} + \sum_{\mathsf{e}\in\mathsf{E}} \int_0^{\ell_\mathsf{e}} f_\mathsf{e}'(x) h_\mathsf{e}'(x)\,\mathrm{d}x \\
&\overset{!}{=} -h(\mathsf{v}) \sum_{\mathsf{e}\sim\mathsf{v}} \frac{\partial f_\mathsf{e}}{\partial n}(\mathsf{v}) + \sum_{\mathsf{e}\in\mathsf{E}} \int_0^{\ell_\mathsf{e}} f_\mathsf{e}'(x) h_\mathsf{e}'(x)\,\mathrm{d}x \\
&\overset{?}{=} \sum_{\mathsf{e}\in\mathsf{E}} \int_0^{\ell_\mathsf{e}} f_\mathsf{e}'(x) h_\mathsf{e}'(x)\,\mathrm{d}x = \mathfrak{a}(f, h)
\end{aligned}$$

Consider

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

and

$$D(\Delta_{\mathcal{G}}) := -\left\{f \in H^1(\mathcal{G}) \cap \bigoplus_{\mathsf{e}\in\mathsf{E}} H^2(0,\ell_{\mathsf{e}}) : \sum_{\mathsf{e}\sim\mathsf{v}} \frac{\partial f_{\mathsf{e}}}{\partial n}(\mathsf{v}) = 0 \ \forall \mathsf{v} \in \mathsf{V}\right\}$$

Proposition (Pavlov–Faddeev 1983, Nicaise 1986)

$\Delta_{\mathcal{G}}$ is a self-adjoint operator on $L^2(\mathcal{G})$ with compact resolvent.

Proof.

- It suffices to prove that $\Delta_{\mathcal{G}}$ is associated with the closed quadratic form $\mathfrak{a}^{\mathcal{G}}(f,g) := \int_{\mathcal{G}} f'(x)g'(x)\,\mathrm{d}x$ with domain $D(\mathfrak{a}^{\mathcal{G}}) := H^1(\mathcal{G})$.
- Already proved: $\Delta_{\mathcal{G}} \subset A$. Exercise: prove $A \subset \Delta_{\mathcal{G}}$.
- $D(\mathfrak{a}^{\mathcal{G}}) = H^1(\mathcal{G}) \subset \bigoplus_{\mathsf{e}\in\mathsf{E}} H^1(0,\ell_{\mathsf{e}}) \overset{c}{\hookrightarrow} \bigoplus_{\mathsf{e}\in\mathsf{E}} L^2(0,\ell_{\mathsf{e}}) = L^2(\mathcal{G})$.

□

Remark

More generally, every bounded elliptic bilinear form $\mathfrak{a}$ on $L^2(\Omega;\mu)$ is associated with an operator that generates an analytic semigroup on $L^2(\Omega;\mu)$; the generator is self-adjoint iff $\mathfrak{a}$ is symmetric.

Spectral properties of $\Delta_{\mathcal{G}}$

$\Delta_{\mathcal{G}}$ has purely point spectrum.
Denote the eigenvalues of $-\Delta_{\mathcal{G}}$ by

$$0 = \lambda_1(\mathcal{G}) \leq \lambda_2(\mathcal{G}) \leq \ldots \nearrow \infty$$

$\lambda_1(\mathcal{G}) < \lambda_2(\mathcal{G})$ iff $\mathcal{G}$ is connected; otherwise, $m(0) = \#$ of connected components of $\mathcal{G}$.

Parabolic properties of $\Delta_{\mathcal{G}}$

$\mathrm{e}^{t\Delta_{\mathcal{G}}}$ solves

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \dfrac{\partial^2 u}{\partial x^2}(t,x) & t \geq 0,\ x \in \mathcal{G} \\ u(t,\cdot) \in C(\mathcal{G}), & \\ \displaystyle\sum_{\mathsf{e}\sim\mathsf{v}} \dfrac{\partial u_{\mathsf{e}}}{\partial n}(t,\mathsf{v}) = 0 & t \geq 0,\ \mathsf{v} \in \mathsf{V}, \\ u(0,x) = u_0(x) & t \geq 0,\ x \in \mathcal{G}. \end{cases}$$

Because $\mathrm{e}^{t\Delta_{\mathcal{G}}}$, it maps $L^2(\mathcal{G})$ to $H^1(\mathcal{G}) \hookrightarrow L^\infty(\mathcal{G})$:

Kantorovič–Wulich $\rightsquigarrow$ $\mathrm{e}^{t\Delta}$ has a kernel of class $L^\infty(\Omega \times \Omega)$ for all $t > 0$.

Markovian property

Spectral Theorem: $\Delta_{\mathcal{G};\mathrm{V^D}}$ generates an analytic semigroup on $L^2(\mathcal{G})$.

Proposition (Kramar–M.–Sikolya 2007)

$(\mathrm{e}^{t\Delta_{\mathcal{G}}})_{t\geq 0}$ *is a Markovian, stochastic semigroup.*
In particular $\int_{\mathcal{G}}\int_{\mathcal{G}} p_t(x,y)\,\mathrm{d}x\,\mathrm{d}y = |\mathcal{G}|$ *for all* $t \geq 0$.
$(\mathrm{e}^{t\Delta_{\mathcal{G}}})_{t\geq 0}$ *satisfies a strong maximum principle iff* $\mathcal{G}$ *is connected*

$\rightsquigarrow$ Feynman–Kac formula holds.
Kostrykin–Potthoff–Schrader 2011: $\Delta_{\mathcal{G}}$ generates a Brownian motion on $\mathcal{G}$.

Proof

- Beurling–Deny 1959: If $A \sim \mathfrak{a}$, and $\mathfrak{a} \geq 0$, then $(\mathrm{e}^{tA})_{t\geq 0}$ is Markovian iff $f \in D(\mathfrak{a})$ implies $f \wedge \mathbf{1} \in D(\mathfrak{a})$ and $\mathfrak{a}(f \wedge \mathbf{1}, (f - \mathbf{1})^+) \geq 0$.
- Ouhabaz 1996: If $A \sim \mathfrak{a}$, and if $(\mathrm{e}^{tA})_{t\geq 0}$ is positive, then $(\mathrm{e}^{tA})_{t\geq 0}$ satisfies the strong maximum principle iff for each measurable $\omega \subset X$ $\mu(\omega) = 0$ or $\mu(X \setminus \omega) = 0$ whenever $\mathbf{1}_\omega f \in D(\mathfrak{a})$ for every $f \in D(\mathfrak{a})$.
- $f_\mathrm{e} \in H^1(0, \ell_\mathrm{e})$ implies $f_\mathrm{e} \wedge \mathbf{1} \in H^1(0, \ell_\mathrm{e})$ and

$$\int_0^{\ell_\mathrm{e}} (f_\mathrm{e} \wedge \mathbf{1})'(x)(f_\mathrm{e} - \mathbf{1})^+)'(x)\,\mathrm{d}x = \int_{\{f\leq 1\}} (f_\mathrm{e} \wedge \mathbf{1})'(x)(f_\mathrm{e} - \mathbf{1})^+)'(x)\,\mathrm{d}x = 0.$$

- Also, $\mathbf{1}_{\omega_\mathrm{e}} f \notin H^1(0, \ell_\mathrm{e}) \hookrightarrow C[0, \ell_\mathrm{e}]$ unless $\omega_\mathrm{e} = \emptyset$ or $\omega_\mathrm{e}(0, \ell_\mathrm{e})$.
- To conclude, observe that $f \in C(\mathcal{G})$ implies $f \wedge \mathbf{1} \in C(\mathcal{G})$.
- Finally $\mathrm{Ker}(\Delta_\mathcal{G}) = \langle \mathbb{1} \rangle$. Hence, $\int_\mathcal{G} p_t(x, y)\,\mathrm{d}y = \mathrm{e}^{t\Delta_\mathcal{G}} \mathbf{1} = \mathbf{1}$ $\forall t \geq 0$.

Dirichlet boundary conditions

Upon imposing Dirichlet conditions on $\mathsf{V}^{\mathrm{D}} \subset \mathsf{V}$, consider the Sobolev space

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

Restricting $\mathfrak{A}^{\mathcal{G}}$ to $H^1(\mathcal{G}; \mathsf{V}^{\mathrm{D}})$ we obtain

- a Laplacian $\Delta_{\mathcal{G};\mathsf{V}^{\mathrm{D}}}$ with eigenvalues

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

- a semigroup $(\mathrm{e}^{t\Delta_{\mathcal{G};\mathsf{V}^{\mathrm{D}}}})_{t\geq 0}$ on $L^2(\mathcal{G})$

Proposition (M. 2007)

$(\mathrm{e}^{t\Delta_{\mathcal{G};\mathsf{V}^{\mathrm{D}}}})_{t\geq 0}$ *is a sub-Markovian, non-stochastic semigroup.*
$(\mathrm{e}^{t\Delta_{\mathcal{G};\mathsf{V}^{\mathrm{D}}}})_{t\geq 0}$ *satisfies a strong maximum principle iff* $\mathcal{G} \setminus \mathsf{V}^{\mathrm{D}}$ *is connected.*

Domination

A C_0-semigroup $(T(t))_{t\geq 0}$ on $L^p(\Omega)$ is said to **dominate** another C_0-semigroup $(S(t))_{t\geq 0}$ if $|S(t)f| \leq T(t)|f|$ for all $f \in L^p(\Omega)$ and all $t \geq 0$.

Proposition

$(\mathrm{e}^{t\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}}})_{t\geq 0}$ *is dominated by* $(\mathrm{e}^{t\Delta_{\mathcal{G}}})_{t\geq 0}$.

Exercise (Diamagnetic inequality for point interactions)

Same holds if magnetic vertex conditions

$$u(\mathsf{v}+) = \mathrm{e}^{i\theta_\mathsf{v}} u(\mathsf{v}-)$$

are imposed on finitely many vertices V^m *of degree 2.*

Given two subspaces U, V of $L^2(\Omega;\mu)$, U is a **generalized ideal** of V if

- $u \in U \Rightarrow |u| \in V$
- $u \in U,\ v \in V,\ |v| \leq |u| \Rightarrow v \operatorname{sgn} u \in U$.

Example

$H^1_{antiper}(0,1)$ is a generalized ideal of $H^1_{per}(0,1)$; neither of them is a generalized ideal of $H^1(0,1)$, but $H^1_0(0,1)$ is.

Proof

- Fact: Ouhabaz 1996: Let $A \sim \mathfrak{a}$, $B \sim \mathfrak{b}$. If $\mathfrak{a}$ is a restriction of $\mathfrak{b}$, and if $(e^{tA})_{t\geq 0}, (e^{tB})_{t\geq 0}$ are both positive, then $(e^{tA})_{t\geq 0}$ dominates $(e^{tB})_{t\geq 0}$ iff $D(\mathfrak{b})$ is a generalized ideal of $D(\mathfrak{a})$.
- No Dirichlet conditions: $\Delta_{\mathcal{G}}$ is associated with the quadratic form

$$\mathfrak{a}(f,g), \qquad f,g \in D(\mathfrak{b}) := H^1(\mathcal{G})$$

  ($\rightsquigarrow$ positive semigroup)
- If Dirichlet conditions are imposed on $\mathrm{V}^{\mathrm{D}} \subset \mathrm{V}$, then the corresponding operator $\Delta_{\mathcal{G};\mathrm{V}^{\mathrm{D}}}$ is associated with

$$\mathfrak{b}(f,g) := \mathfrak{a}(f,g), \qquad f,g \in D(\mathfrak{b}) := H^1_0(\mathcal{G};\mathrm{V}^{\mathrm{D}})$$

  where $H^1_0(\mathcal{G};\mathrm{V}^{\mathrm{D}}) := \{f \in H^1(\mathcal{G}) : f(\mathrm{v}) = 0\ \forall \mathrm{v} \in \mathrm{V}^{\mathrm{D}}\}$.
- Let us check Ouhabaz' criterion: $H^1_0(\mathcal{G};\mathrm{V}^{\mathrm{D}})$ is a generalized ideal of $H^1(\mathcal{G})$: $f \in H^1_0(\mathcal{G};\mathrm{V}^{\mathrm{D}}) \Rightarrow |f| \in H^1(\mathcal{G})$; and $|g| \leq |f|$ with $f \in H^1_0(\mathcal{G};\mathrm{V}^{\mathrm{D}}) \Rightarrow$ $g \operatorname{sgn} f \in H^1_0(\mathcal{G};\mathrm{V}^{\mathrm{D}})$.

Theorem (Kramar–M.–Sikolya 2007, M.–Romanelli 2007, Bifulco–M. 2023)

Given $\mathcal{G}$ on finitely many edges of finite length, the Laplacian $\Delta_{\mathcal{G}}$ on $\mathcal{G}$ is associated with a heat kernel $p^{\mathcal{G}} = p_t^{\mathcal{G}}(x,y)$ that satisfies

- $0 \leq p_t^{\mathcal{G}}(x,y) \leq 1$ *for all* t *and all* $x, y \in \mathcal{G}$;
- *if* $\mathcal{G}$ *is connected,* $0 < p_t^{\mathcal{G}}(x,y)$ *for all* t *and all* $x, y \in \mathcal{G}$;
- $\int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G}}(x,y)\,\mathrm{d}x\,\mathrm{d}y = |\mathcal{G}|$ *for all* $t > 0$.
- *if Dirichlet conditions are imposed on a subset* $\mathrm{V}^{\mathrm{D}} \subset \mathcal{G}$, $p_t^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}(x,y) \leq p_t^{\mathcal{G}}(x,y)$;
- *both* $p_t^{\mathcal{G}}$ *and* $\frac{\partial^2}{\partial x^2}\frac{\partial^2}{\partial y^2} p_t^{\mathcal{G}}$ *are jointly Lipschitz continuous, but* $p_t^{\mathcal{G}}(\cdot, y)$ *is not continuously differentiable for any* y *unless* $\mathcal{G}$ *is a loop or a path.*

Smoothness of functions in $D(\Delta_{\mathcal{G}})$

Lemma (M.–Plümer 2023)

$D(\Delta_{\mathcal{G}})$ is continuously embedded in $\mathrm{Lip}(\mathcal{G})$.

Proof.

- $D(\Delta_{\mathcal{G}}) \hookrightarrow C(\mathcal{G}) \cap \bigoplus_{e \in E} H^2(0, \ell_e) \hookrightarrow C(\mathcal{G}) \cap \bigoplus_{e \in E} W^{1,\infty}(0, \ell_e)$.
- Let $u \in C(\mathcal{G}) \cap \bigoplus_{e \in E} W^{1,\infty}(0, \ell_e)$. Let $x, y \in \mathcal{G}$ and let $\gamma \subset \mathcal{G}$ be a path connecting x and y. Then
$$|u(x) - u(y)| = \left| \int_\gamma u'(t)\,\mathrm{d}t \right| \leq \mathrm{length}(\gamma) \|u'\|_\infty .$$
- γ arbitrary $\Rightarrow$
$$|u(x) - u(y)| \leq \|u'\|_\infty d^{\mathcal{G}}(x, y).$$
Therefore, $C(\mathcal{G}) \cap \bigoplus_{e \in E} W^{1,\infty}(0, \ell_e) \hookrightarrow \mathrm{Lip}(\mathcal{G})$.

□

In particular: eigenfunctions of $\Delta_{\mathcal{G}}$ are Lipschitz continuous (but not continuously differentiable!).

Theorem (Kramar–M.–Sikolya 2007, M.–Romanelli 2007, Bifulco–M. 2023)

Given $\mathcal{G}$ on finitely many edges of finite length, the Laplacian $\Delta_{\mathcal{G}}$ on $\mathcal{G}$ is associated with a heat kernel $p^{\mathcal{G}} = p_t^{\mathcal{G}}(x,y)$ that satisfies

- $0 \le p_t^{\mathcal{G}}(x,y)$, $\int : \mathcal{G} p_t(x,z)\,\mathrm{d}z = 1$ *for all* t *and all* $x, y \in \mathcal{G}$;
- *if* $\mathcal{G}$ *is connected,* $0 < p_t^{\mathcal{G}}(x,y)$ *for all* t *and all* $x, y \in \mathcal{G}$;
- $\int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G}}(x,y)\,\mathrm{d}x\,\mathrm{d}y = |\mathcal{G}|$ *for all* $t > 0$;
- *if Dirichlet conditions are imposed on a subset* $\mathrm{V}^{\mathrm{D}} \subset \mathcal{G}$, $p_t^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}(x,y) \le p_t^{\mathcal{G}}(x,y)$;
- *both* $p_t^{\mathcal{G}}$ *and* $\frac{\partial^2}{\partial x^2}\frac{\partial^2}{\partial y^2} p_t^{\mathcal{G}}$ *are jointly Lipschitz continuous, but* $p_t^{\mathcal{G}}(\cdot, y)$ *is not continuously differentiable for any* y *unless* $\mathcal{G}$ *is a loop or a path.*

Hence by Mercer:

$$p_t^{\mathcal{G}}(x,y) = \sum_{n \in \mathbb{N}} \lambda_n \varphi_n(x)\varphi_n(y) \qquad \text{for all } t > 0,\ x, y \in \mathcal{G}.$$

(uniform convergence)

Open question: Convergence in Lipschitz norm, too? H^1-norm?

Proof based on

Theorem (Bifulco–M. 2023)

Let A be self-adjoint and generate an analytic semigroup $(\mathrm{e}^{tA})_{t\geq 0}$ on $L^2(X,\mu)$ s.t. $D(A^k) \hookrightarrow C^{0,\alpha}(X)$ for some $k \in \mathbb{N}$ and some $\alpha \in (0,1]$.
Then there exists a pointwise heat kernel $p = p_\cdot(\cdot,\cdot)$ s.t. $p_t(\cdot,\cdot), A_x A_y p_t(\cdot,\cdot)$ is α-Hölder continuous for all $t > 0$.

More general operators

Proposition

Everything we have seen is still valid if Δ is replaced by

$$A_{c,V,\gamma}u := \frac{\partial}{\partial x}\left(c(\cdot)\frac{\partial}{\partial x}\right) + V$$

with "δ-interaction"

$$\text{continuity} \quad + \quad \sum_{\mathsf{e}\sim\mathsf{v}} c_{\mathsf{e}}(\mathsf{v})\frac{\partial u_{\mathsf{e}}}{\partial n}(\mathsf{v}) + \gamma(\mathsf{v})u(\mathsf{v}) = 0$$

for $c \in L^\infty(\mathcal{G})$, $V \in L^1(\mathcal{G})$, and $(\gamma(\mathsf{v}))_{\mathsf{v}\in\mathsf{V}}$.

Proof.

$A_{c,V,\gamma}$ is associated with

$$\mathfrak{a}^{\mathcal{G}}_{c,V,\gamma}(f) := \int_{\mathcal{G}} a(x)|f'(x)|^2\,\mathrm{d}x + \int_{\mathcal{G}} V(x)|f(x)|^2\,\mathrm{d}x + \sum_{\mathsf{v}\in\mathsf{V}}\gamma(\mathsf{v})|f(\mathsf{v})|^2$$

with same form domain $D(\mathfrak{a}^{\mathcal{G}}_{c,V,\gamma}(f)) = D(\mathfrak{a}^{\mathcal{G}}) = H^1(\mathcal{G})$. □

! Dirichlet conditions at a vertex can be obtained letting $\gamma(\mathsf{v}) \to +\infty$.

Lack of domination

Proposition

If $\mathcal{G}, \mathcal{G}'$ any two different wirings over the same edge set, then $\mathrm{e}^{t\Delta_{\mathcal{G}}}$ does not dominate $\mathrm{e}^{t\Delta_{\mathcal{G}'}}$ for any $t > 0$.

Proof.

$D(\mathfrak{a}^{\mathcal{G}})$ is not a generalized ideal of $D(\mathfrak{a}^{\mathcal{G}'})$ (Exercise) □

Miscellaneous comments

- Kennedy–Lang 2020: Similar results also hold operators with $V \in L^1(\mathcal{G};\mathbb{C})$, $(\gamma(\mathsf{v}))_{\mathsf{v}\in\mathsf{V}} \subset \mathbb{C}$. In particular, $|\mathrm{e}^{tA_{c,V,\gamma}}| \le \mathrm{e}^{tA_{c,\mathrm{Re}\,V,\mathrm{Re}\,\gamma}}$
- Kurasov 2010, Berkolaiko–Weyand 2012, Egidi–M.–Seelmann 2023: One can also add a magnetic potential: somewhat trivial, because a gauge transformation makes Δ_α similar to Δ. A diamagnetic inequality holds:

$$|\mathrm{e}^{t\Delta_\alpha}| \le \mathrm{e}^{t\Delta} \qquad \text{for all } t > 0.$$

- Glück–M. 2021: If $\mathcal{G}, \mathcal{G}'$ any two different wirings over the same edge set, then $\mathrm{e}^{t\Delta_{\mathcal{G}}}$ does not even *eventually* dominate $\mathrm{e}^{t\Delta_{\mathcal{G}'}}$:
  there is no $t_0 > 0$ such that $\mathrm{e}^{t\Delta_{\mathcal{G}}} \le \mathrm{e}^{t\Delta_{\mathcal{G}'}}$ for all $t > t_0$.

  Open question: Given two different wirings $\mathcal{G}, \mathcal{G}'$, is there $M > 0$ such that $\mathrm{e}^{t\Delta_{\mathcal{G}}} \le M\mathrm{e}^{t\Delta_{\mathcal{G}'}}$ for all $t > 0$?

Extension #1: Different boundary conditions

Consider boundary conditions of type

$$A\underline{f} + B\underline{\underline{f}} = 0$$

where

$$\underline{f} := \begin{pmatrix} f_{e_1}(0) \\ \vdots \\ f_{e_{\#E}}(0) \\ f_{e_1}(\ell_e) \\ \vdots \\ f_{e_{\#E}}(\ell_{\#E}) \end{pmatrix} \qquad \underline{\underline{f}} := \begin{pmatrix} f'_{e_1}(0) \\ \vdots \\ f'_{e_{\#E}}(0) \\ f'_{e_1}(\ell_e) \\ \vdots \\ f'_{e_{\#E}}(\ell_{\#E}) \end{pmatrix}$$

Theorem (Cardanobile–M. 2009; Kurasov 2019)

Only "continuous"-like vertex conditions ($\underline{f} \equiv f_{|V}$) induce a positive semigroup.

Theorem (Hussein–M. 2020)

Let $A, B \in M_2(\mathbb{C})$. *Assume the zero* k *of* $\{k : \operatorname{Im} k > 0\} : k \mapsto \det(A + ikB) \in \mathbb{C}$ *of larger magnitude lies on* $i(0, \infty)$, *and let* $A \neq \kappa_0 B$ *and*

$$\lim_{\kappa \searrow \kappa_0} \frac{(\kappa - \kappa_0)^2}{\det(A - \kappa B)} = 0$$

Then $\mathrm{e}^{t\Delta}$ *is asymptotically eventually positive.*

Example

Let $\mathcal{G} \equiv \mathbb{R}$. *Then*

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \dfrac{\partial^2 u}{\partial x^2}(t,x) & t \geq 0,\ x \in \mathcal{G}, \\ u'(t,0+) = u(t,0-), & t \geq 0, \\ u'(t,0-) = u(t,0+), & t \geq 0, \\ \quad u(0,x) = u_0(x) & x \in \mathcal{G}. \end{cases}$$

is governed by an analytic semigroup on $L^2(\mathcal{G})$ *that is not positive; however, it is asymptotically positive.*

Extension #2: enlarging the Hillbert space

$$H^1(\mathcal{G}) \equiv \mathbb{H}^1(\mathcal{G}) := \left\{ \begin{pmatrix} f \\ f_{|\mathsf{V}} \end{pmatrix} \in L^2(\mathcal{G}) \oplus \mathbb{R}^{\mathsf{V}} : f \in H^1(\mathcal{G}) \right\} \hookrightarrow L^2(\mathcal{G}) \oplus \mathbb{R}^{\mathsf{V}} =: \mathbb{L}^2(\mathcal{G})$$

Consider

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

and the operator $\mathbb{A}_{\mathcal{G}}$ associated with $\mathfrak{A}^{\mathcal{G}}$ in $\mathbb{L}^2(\mathcal{G})$.

Diffusion with dynamic boundary conditions

Theorem (M.–Romanelli 2007)

$\mathbb{\Delta}_{\mathcal{G}}$ *is a self-adjoint operator with compact resolvent.*
$\mathrm{e}^{t\mathbb{\Delta}_{\mathcal{G}}}$ *solves*

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \dfrac{\partial^2 u}{\partial x^2}(t,x) & t \geq 0,\ x \in \mathcal{G}, \\ u(t,\cdot) \in C(\mathcal{G}), & \\ \dfrac{\partial u}{\partial t}(t,\mathrm{v}) = -\displaystyle\sum_{\mathrm{e}\sim\mathrm{v}} \dfrac{\partial u_{\mathrm{e}}}{\partial n}(t,\mathrm{v}) & t \geq 0,\ \mathrm{v} \in \mathrm{V}, \\ u(0,x) = u_0(x) & t \geq 0,\ x \in \mathcal{G}. \end{cases}$$

$\mathrm{e}^{t\mathbb{\Delta}_{\mathcal{G}}}$ *is a* **Markovian, stochastic** *semigroup.*

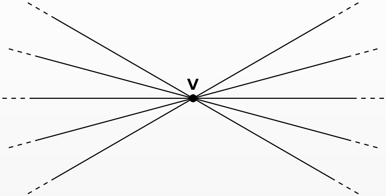
Kostrykin–Potthoff–Schrader 2012; Bonaccorsi–D'Ovidio 2024: $\mathbb{\Delta}_{\mathcal{G}}$ generates a sticky Brownian motion on $\mathcal{G}$.

Extension #3: modifying the metric measure structure ("tilting")

Let $\mathcal{G}$ be a star graph, $\ell_e \equiv \infty$.

Unless otherwise mentioned:

- ~~$d \equiv$ *Euclidean distance*~~
- ~~$d \equiv$ *Lebesgue measure*~~



In this case: endowing each edge with

- arctan-distance: $d_{\text{arctan}}(x, y) = |\arctan(x) - \arctan(y)|$
- Gaussian measure: $\mathrm{d}\mu(x) := \mathrm{e}^{-x^2}\,\mathrm{d}x$

$\mathcal{G}$ is a metric space with finite diameter and finite measure: then

- $H^1(\mathcal{G}) \overset{\text{(Carlson 2000)}}{\hookrightarrow} C^{0,\frac{1}{2}}(\overline{\mathcal{G}}) \overset{c}{\hookrightarrow} C(\overline{\mathcal{G}}) \hookrightarrow L^\infty(\mathcal{G}) \hookrightarrow L^2(\mathcal{G})$.

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

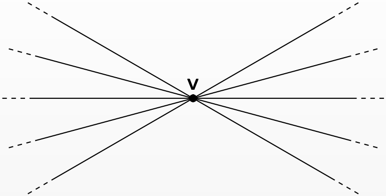
and the operator $A^{\mathcal{G}}_{OU}$ associated with $\mathfrak{A}^{\mathcal{G}}$ in $L^2(\mathcal{G})$.

Extension #3: modifying the metric measure structure ("tilting")

Let $\mathcal{G}$ be a star graph, $\ell_e \equiv \infty$.

Unless otherwise mentioned:

- ~~$d \equiv$ Euclidean distance~~
- ~~$d \equiv$ Lebesgue measure~~



In this case: endowing each edge with

- arctan-distance: $d_{\text{arctan}}(x,y) = |\arctan(x) - \arctan(y)|$
- Gaussian measure: $\mathrm{d}\mu(x) := \mathrm{e}^{-x^2}\,\mathrm{d}x$

$\mathcal{G}$ is a metric space with finite diameter and finite measure: then

- $H^1(\mathcal{G}) \overset{\text{(Carlson 2000)}}{\hookrightarrow} C^{0,\frac{1}{2}}(\overline{\mathcal{G}}) \overset{c}{\hookrightarrow} C(\overline{\mathcal{G}}) \hookrightarrow L^\infty(\mathcal{G}) \hookrightarrow L^2(\mathcal{G})$.

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

and the operator $A^{\mathcal{G}}_{OU}$ associated with $\mathfrak{A}^{\mathcal{G}}$ in $L^2(\mathcal{G})$.

Extension #2: the Ornstein–Uhlenbeck operator

Theorem (M.–Rhandi 2022)

$A_{OU}^{\mathcal{G}}$ is self-adjoint in $L^2(\mathcal{G})$ with compact resolvent[a].

$\mathrm{e}^{tA_{OU}^{\mathcal{G}}}$ solves

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) = \dfrac{\partial^2 u}{\partial x^2}(t,x) - 2|x|\dfrac{\partial u}{\partial x}(t,x) & t \geq 0,\ x \in \mathcal{G}, \\ u(t,\cdot) \in C(\mathcal{G}), & \\ \displaystyle\sum_{\mathrm{e}\sim\mathrm{v}} \dfrac{\partial u_{\mathrm{e}}}{\partial n}(t,\mathrm{v}) = 0 & t \geq 0,\ \mathrm{v} \in \mathrm{V}, \\ u(0,x) = u_0(x) & t \geq 0,\ x \in \mathcal{G}. \end{cases}$$

$\mathrm{e}^{tA_{OU}}$ is a **Markovian, stochastic** *semigroup.*

[a] Both false if Lebesgue measure is considered instead!!!

$A_{OU}^{\mathcal{G}}$ generates an Ornstein–Uhlenbeck process on $\mathcal{G}$.

Extension #3: Flows of different functionals in different metric spaces

Recall:

- The **Laplacian** $\Delta_{\mathcal{G}}$ on $\mathcal{G}$ is associated with the quadratic form

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

- Equivalently: the heat equation driven by $\Delta_{\mathcal{G}}$ on $L^2(\mathcal{G})$ is the gradient flow for $\mathfrak{A}^{\mathcal{G}}$ wrt metric of $L^2(\mathcal{G})$.
- The associated semigroup $\mathrm{e}^{t\Delta_{\mathcal{G}}}$ is Markovian whenever standard conditions are imposed at each $\mathsf{v} \in \mathsf{V}$, i.e., up to changing $\sim$ with another equivalence relation: i.e., whenever Neumann or continuity+Kirchhoff conditions are imposed.

Example

If $\mathcal{G}$ consists of one edge, $\mathrm{e}^{t\Delta_{\mathcal{G}}}$ is Markovian precisely for periodic BCs ($\mathcal{G} \equiv$ loop) or Neumann BCs ($\mathcal{G} \equiv$ path)

Theorem (Jordan–Kinderlehrer–Otto 1998)

The gradient flow of

$$\mathfrak{a}(f) := \frac{1}{2}\int_{\mathbb{R}^d} |\nabla f|^2 \, \mathrm{d}x$$

wrt $L^2(\mathbb{R}^d)$*-metric and the gradient flow of*

$$\mathcal{E}(\rho) := \int_{\mathbb{R}^d} \rho \log \rho \, \mathrm{d}\rho$$

wrt Wasserstein metric

$$W_2(\mu,\nu) := \min_{\sigma\in\Pi(\mu,\nu)} \left(\int_{\mathbb{R}^d\times\mathbb{R}^d} \mathrm{dist}^2(x,y)\, \mathrm{d}\sigma(x,y) \right)^{\frac{1}{2}}$$

coincide.

($\Pi(\mu,\nu) \equiv$ set of probability measures on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals μ,ν)

More precisely:
$\mathcal{E}$ induces a time-discrete iterative variational scheme whose solutions converge (weakly in $L^1(\mathbb{R}^d)$) to the solution of the heat equation.

Goal: represent

$$\frac{\partial \eta}{\partial t} = \Delta \eta$$

as the gradient flow wrt W_2 of the **relative entropy**

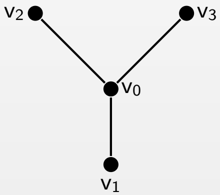
$$\mathcal{E}(\mu) := \begin{cases} \int_{\mathcal{G}} \eta(x) \log \eta(x) \, \mathrm{d}\lambda(x) & \text{if } \mu = \eta\lambda, \quad (\lambda \equiv \text{Lebesgue}) \\ +\infty & \text{otherwise} \end{cases}$$

Branching of geodesics

A metric space (X, d) is **non-branching** if for any two geodesics $\gamma^1, \gamma^2 : [0,1] \to X$

$$\gamma_0^1 = \gamma_0^2 \text{ and } \gamma_{t_0}^1 = \gamma_{t_0}^2 \text{ for some } t_0 \Rightarrow \gamma_t^1 = \gamma_t^2 \text{ for all } t \in [0,1].$$

Problem: In a metric graph there may exist distinct geodesics $\gamma, \tilde{\gamma} : [0,1] \to \mathcal{G}$ that agree on an open subset of $[0,1]$.



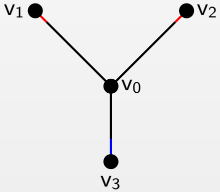
Think of the (constant-speed!) geodesics connecting v_1 with v_2, resp., v_1 with v_3.

Branching of geodesics

A metric space (X, d) is **non-branching** if for any two geodesics $\gamma^1, \gamma^2 : [0,1] \to X$

$$\gamma^1_0 = \gamma^2_0 \text{ and } \gamma^1_{t_0} = \gamma^2_{t_0} \text{ for some } t_0 \Rightarrow \gamma^1_t = \gamma^2_t \text{ for all } t \in [0,1].$$

Problem: In a metric graph there may exist distinct geodesics $\gamma, \tilde{\gamma} : [0,1] \to \mathcal{G}$ that agree on an open subset of $[0,1]$.



Lemma (Erbar–Forkert–Maas–M. 2022)

The relative entropy of the optimal coupling of μ and ν is piecewise affine $\rightsquigarrow$ NOT geodesically convex.

⚠ Uniqueness???

- $\mathcal{G}$ is a geodesic space $\overset{\text{Lisini 2006}}{\rightsquigarrow}$ $\mathcal{P}(\mathcal{G})$ is a geodesic space
- $\mathcal{E}$ is lsc on $(\mathcal{P}(\mathcal{G}); W_2)$, but
- $\mathcal{E}$ is NOT geodesically convex, and
- still need to extend Benamou–Brenier to metric graphs.

- $\mathcal{G}$ is a geodesic space $\overset{\text{Lisini 2006}}{\rightsquigarrow}$ $\mathcal{P}(\mathcal{G})$ is a geodesic space
- $\mathcal{E}$ is lsc on $(\mathcal{P}(\mathcal{G}); W_2)$,but
- $\mathcal{E}$ is NOT geodesically convex, and
- still need to extend Benamou–Brenier to metric graphs.

A dynamic formulation of Wasserstein

Theorem (Benamou–Brenier 2000)

For all probability measures μ, ν on $\mathbb{R}^d$ with finite second moment

$$W_2(\mu,\nu) = \inf_{(\mu_t, v_t)} \left(\int_0^1 \|v_t\|^2_{L^2(\mu_t)} \, \mathrm{d}t \right)^{\frac{1}{2}}$$

Infimum taken over all curves $\mu_\cdot : [0,1] \to (\mathcal{P}(\mathbb{R}^d); W_2)$ s.t. (μ_t, v_t) solves

$$\begin{cases} \dfrac{\partial \mu_t}{\partial t} = \nabla \cdot (v_t \mu_t), & t \in [0,1], \\ \mu_0 = \mu, \\ \mu_1 = \nu. \end{cases}$$

A dynamic formulation of Wasserstein on metric graphs

Theorem (Erbar–Forkert–Maas–M. 2022)

For all probability measures μ, ν on $\mathcal{G}$ ~~with finite second moment~~

$$W_2(\mu, \nu) = \inf_{(\mu_t, v_t)} \left(\int_0^1 \|v_t\|^2_{L^2(\mu_t)} \, \mathrm{d}t \right)^{\frac{1}{2}}$$

Infimum taken over all curves $\mu_\cdot : [0,1] \to (\mathcal{P}(\mathcal{G}); W_2)$ s.t. (μ_t, v_t) is weak solution of

$$\begin{cases} \dfrac{\partial \mu_t}{\partial t} = \nabla \cdot (v_t \mu_t), & t \in [0,1], \\ \mu_0 = \mu, \\ \mu_1 = \nu \end{cases}$$

A JKO-type scheme

Theorem (Erbar–Forker–Mass–M. 2022)

For any probability measure μ_0 *on* $\mathcal{G}$ *and any* $\tau > 0$, *the variational scheme*

$$\mu_0^\tau := \mu_0$$
$$\mu_n^\tau := \operatorname{argmin}_\nu \left(\mathcal{E}(\nu) + \frac{1}{2\tau} W_2(\nu, \mu_{n-1}^\tau)^2 \right)$$

has a solution. Define a piecewise constant curve

$$\bar{\mu}_0^\tau := \mu_0$$
$$\bar{\mu}_t^\tau := \mu_n^\tau \quad \textit{if } t \in ((n-1)t, nt].$$

As $\tau \to 0$ *there exists a subsequence* $(\mu_t^{\tau_k})_k$ *that weakly converges to a "weak solution* μ_t*" of the heat equation on* $\mathcal{G}$.

Extension to McKean–Vlasov processes

Given

$$V \in \bigoplus_{e \in E} \mathrm{Lip}(0, \ell_e) \qquad\qquad W \in \mathrm{Lip}(\mathcal{G} \times \mathcal{G}) \text{ and symmetric :}$$

drift — interaction

Represent (Fokker–Planck equation of a McKean–Vlasov process!)

$$\frac{\partial \eta}{\partial t} = \Delta\eta + \nabla \cdot \big(\eta\big(\nabla V + \nabla W[\mu]\big)\big) \qquad (\mu = \eta e^{-V}\lambda,\ \lambda = \text{Lebesgue})$$

as the gradient flow wrt W_2 of

$$\mathcal{F}(\mu) := \begin{cases} \displaystyle\int_{\mathcal{G}} \eta(x) \log \eta(x)\, \mathrm{d}\lambda(x) + \int_{\mathcal{G}} V(x)\eta(x)\, \mathrm{d}\lambda(x) \\ \displaystyle\qquad + \frac{1}{2}\int_{\mathcal{G}\times\mathcal{G}} W(x,y)\eta(x)\eta(y)\, \mathrm{d}\lambda(x)\, \mathrm{d}\lambda(y), & \text{if } \mu = \eta e^{-V}\lambda, \\ +\infty & \text{otherwise.} \end{cases}$$

Theorem (Erbar–Forkert–Maas–M. 2022)

A JKO-like convergence holds: the W_2-gradient of $\mathcal{F}$ induces a variational scheme that converges to a weak solution of the Vlasov–McKean equation. Also,

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t}(\mu_t) = -\int_{\mathcal{G}} \left| \frac{\nabla \rho_t}{\rho_t} + \nabla W[\mu_t] \right|^2 \mathrm{d}\mu_t .$$

Asymptotic expansions in $\mathbb{R}^d$ for the heat kernel p with Dirichlet BCs

On bounded, open $\Omega \subset \mathbb{R}^d$: **heat trace** $\mathrm{Tr}(\mathrm{e}^{t\Delta})$ and **heat content** $\mathcal{Q}_t(\Omega)$ satisfy asymptotic expansions.

Theorem (Minakshisundaram–Pleijel 1949)

$$\mathrm{Tr}(\mathrm{e}^{t\Delta}) := \int_\Omega p_t(x,x)\,\mathrm{d}x \asymp \frac{1}{(4\pi t)^{\frac{d}{2}}} \sum_{j=0}^{\infty} \alpha_j t^j \qquad \text{as } t \searrow 0$$

Theorem (van den Berg–Davies 1989)

$$\mathcal{Q}_t(\Omega) := \int_{\Omega\times\Omega} p_t(x,y)\,\mathrm{d}x\,\mathrm{d}y \asymp \sum_{j=0}^{\infty} \beta_j t^{\frac{j}{2}} \qquad \text{as } t \searrow 0$$

Here $\alpha_0 = \beta_0 = |\Omega|$, $\alpha_1 = \frac{\sqrt{\pi}}{2}|\partial\Omega|$, $\beta_1 = \frac{2}{\sqrt{\pi}}|\partial\Omega|$; further terms encode geometry of $\partial\Omega$, many are known (van den Berg–Gilkey 1994)

Sketch of the proofs

- Trace formula: Use Hadamard's parametrix method to find an approximate formula for the heat kernel.
- Heat content formula: Apply probabilistic interpretation of the the heat kernel wrt Brownian motion

Asymptotic expansions in $\mathcal{G}$

Theorem (Roth 1984, Nicaise 1986)

$$\mathrm{Tr}(\mathrm{e}^{t\Delta_{\mathcal{G}}}) := \int_\Omega p_t^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}(x,x)\,\mathrm{d}x$$
$$\asymp \frac{1}{2\sqrt{\pi t}} \sum_{j=0}^{\infty} \alpha_j t^j \qquad \text{as } t \searrow 0$$

Theorem (Bifulco–M. 2025)

$$\mathcal{Q}_t(\mathcal{G};\mathrm{V}^{\mathrm{D}}) := \int_{\Omega\times\Omega} p_t^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}(x,y)\,\mathrm{d}x\,\mathrm{d}y$$
$$\asymp \sum_{j=0}^{\infty} \beta_j t^{\frac{j}{2}} \qquad \text{as } t \searrow 0$$

Here $\alpha_0 = \beta_0 = |\mathcal{G}|$, $\alpha_1 = \frac{\sqrt{\pi}}{2}(\#\mathrm{V} - \#\mathrm{V}^{\mathrm{D}} - \#\mathrm{E})$, $\beta_1 = \frac{2}{\sqrt{\pi}}\#\mathrm{V}^{\mathrm{D}}$; no further nontrivial terms exist in general (Kurasov–Nowaczyk 2005; Bifulco–M. 2025)

Sketch of the proofs

- Trace formula (equilateral case): explicit formula for the eigenvalues + Poisson summation formula
- Trace formula (general case): based on explicit construction of the heat kernel of $(\mathrm{e}^{t\Delta_{\mathcal{G}}})_{t\geq 0}$ actually available, via parametrix.

Proposition (Roth 1984)

The heat kernel $p^{\mathcal{G}}$ associated with $\Delta_{\mathcal{G}}$ is given by

$$p_t^{\mathcal{G}}(x,y) := \frac{1}{\sqrt{4\pi t}} \sum_{\gamma \in \mathcal{P}_{x,y}} \alpha(\gamma) \mathrm{e}^{-\frac{\mathrm{length}(\gamma)^2}{4t}}$$

for appropriate "scattering coefficients" $\alpha(\gamma) \in [-1,1]$.

- Heat content formula: Roth's formula for the heat kernel + **heavy** combinatorics

Sketch of the proofs

- Trace formula (equilateral case): explicit formula for the eigenvalues + Poisson summation formula
- Trace formula (general case): based on explicit construction of the heat kernel of $(\mathrm{e}^{t\Delta_{\mathcal{G}}})_{t\geq 0}$ actually available, via parametrix.

Proposition (Roth 1984)

The heat kernel $p^{\mathcal{G}}$ associated with $\Delta_{\mathcal{G}}$ is given by

$$p_t^{\mathcal{G}}(x,y) := \frac{1}{\sqrt{4\pi t}} \sum_{\gamma \in \mathcal{P}_{x,y}} \alpha(\gamma) \mathrm{e}^{-\frac{\mathrm{length}(\gamma)^2}{4t}}$$

for appropriate "scattering coefficients" $\alpha(\gamma) \in [-1,1]$.

- Heat content formula: Roth's formula for the heat kernel + **heavy** combinatorics

Heat content formula & Caccioppoli-type formula

Corollary (Bifulco–M. 2025)

$$\left|\mathcal{Q}_t(\mathcal{G};\mathrm{V}^{\mathrm{D}}) - |\mathcal{G}| - \frac{2\sqrt{t}}{\sqrt{\pi}}\#\mathrm{V}^{\mathrm{D}}\right| \asymp O(t) \quad \text{as } t \searrow 0.$$

Corollary (Bifulco–M. 2025)

If $\mathcal{H}$ is a closed and connected subset of $\mathcal{G}\setminus\mathrm{V}^{\mathrm{D}}$ whose boundary in $\mathcal{G}$ does not contain any vertices of $\mathcal{G}$ of degree ≥ 3, then

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

(For domains in $\mathbb{R}^d$: Miranda Jr–Pallara–Paronetto–Preunkert 2007)

Long-time behavior

Recall: $\Delta_{\mathcal{G}}$ has an ONB of eigenfunctions (φ_k) with associated eigenvalues $-\lambda_k = -\lambda_k(\mathcal{G}) \geq 0$.

If $\mathcal{G}$ is connected, then $\lambda_1 = 0$ (simple!) with $\varphi_1 = \mathbf{1}_{\mathcal{G}}$.

Because $\mathrm{e}^{t\Delta_{\mathcal{G}}} f(\cdot) = \sum_{k=0}^{\infty} \mathrm{e}^{-t\lambda_k} \varphi_k(\cdot) \int_{\mathcal{G}} \varphi_k(x) f(x) \, \mathrm{d}x$,

$$\|\mathrm{e}^{t\Delta_{\mathcal{G}}} f - \int_{\mathcal{G}} f(x) \, \mathrm{d}x\| \leq \mathrm{e}^{-t\lambda_2} \|f\|$$

Estimating λ_2 is crucial to study the long-time behaviour!

Interplays between λ_1 and heat kernel

$$\lim_{t\to\infty} \frac{\log p_t^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}(x,y)}{t} = -\lambda_1(\mathcal{G};\mathrm{V}^{\mathrm{D}}) \qquad \text{holds for all } x,y \in \mathcal{G},$$

(applying Keller–Lenz–Vogt–Wojciechowski 2015)

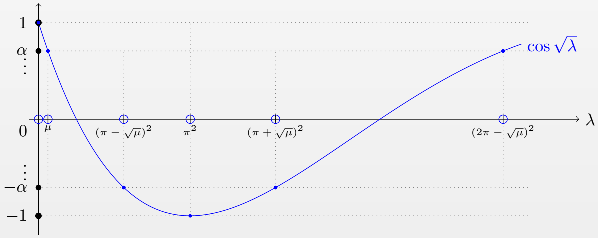
Not aware of estimates on λ_2 based on heat kernel methods, but...

Given $\mathcal{G}$, consider the underlying combinatorial graph G, its degree matrix $\mathcal{D}^{\mathsf{G}}$ and its discrete Laplacian $\mathcal{L}^{\mathsf{G}}$.

Proposition (von Below 1985)

If all $\ell_{\mathsf{e}} \equiv \ell$, TFAE:

- λ *is eigenvalue of* $-\Delta_{\mathcal{G}}$
- $\alpha := \cos\sqrt{\lambda}$ *is eigenvalue of* $\mathrm{Id} - \mathcal{D}_{\mathsf{G}}{}^{-\frac{1}{2}} \mathcal{L}_{\mathsf{G}} \mathcal{D}_{\mathsf{G}}{}^{-\frac{1}{2}}$



Nicaise' Isoperimetric Inequality

Theorem (Nicaise 1987)

For any metric graph $\mathcal{G}$ on finitely many edges of finite length $\lambda_2(\mathcal{G}) \geq \frac{\pi^2}{|\mathcal{G}|^2}$, *with equality if* $\mathcal{G}=$ 

Theorem (Friedlander 2005)

Nicaise' Inequality is sharp. Indeed

$$\lambda_j(\mathcal{G}) \geq \frac{\pi^2 j^2}{4|\mathcal{G}|^2} \qquad \text{for all } j = 2, 3, \ldots,$$

with equality if (and only if!) $\mathcal{G}$ *is a metric star on* j *edges of same length.*

Exercise (Nicaise 1987)

Prove the estimate $\lambda_1(\mathcal{G}; \mathrm{V}^{\mathrm{D}}) \geq \frac{\pi^2}{4|\mathcal{G}|^2}$ *if* $\mathrm{V}^{\mathrm{D}} \neq \emptyset$, *with equality iff* $\mathcal{G}=$ .

Nicaise' Isoperimetric Inequality

Theorem (Nicaise 1987)

For any metric graph $\mathcal{G}$ on finitely many edges of finite length $\lambda_2(\mathcal{G}) \geq \frac{\pi^2}{|\mathcal{G}|^2}$, *with equality if* $\mathcal{G}=$ 

Theorem (Friedlander 2005)

Nicaise' Inequality is sharp. Indeed

$$\lambda_j(\mathcal{G}) \geq \frac{\pi^2 j^2}{4|\mathcal{G}|^2} \qquad \text{for all } j = 2, 3, \ldots,$$

with equality if (and only if!) $\mathcal{G}$ *is a metric star on* j *edges of same length.*

Exercise (Nicaise 1987)

Prove the estimate $\lambda_1(\mathcal{G}; \mathrm{V}^{\mathrm{D}}) \geq \frac{\pi^2}{4|\mathcal{G}|^2}$ *if* $\mathrm{V}^{\mathrm{D}} \neq \emptyset$, *with equality iff* $\mathcal{G}=$ .

Proof of Nicaise' Inequality – Kurasov–Naboko's version

- Produce $\mathcal{G}_{(2)}$ by replacing each edge e in $\mathcal{G}$ by two identical copies of e: then $|\mathcal{G}_{(2)}| = 2|\mathcal{G}|$.
- Take (λ_2, φ_2) and clone φ_2 to produce an admissibile test function $\varphi_2^{(2)}$ for $\lambda_2(\mathcal{G}_{(2)})$: observe that $\varphi_2^{(2)} \perp \mathbf{1}_{\mathcal{G}_{(2)}}$.
- Also, $\|\varphi_2^{(2)}\|^2_{L^2} = 2\|\varphi_2\|^2_{L^2}$, $\|\varphi_2^{(2)'}\|^2_{L^2} = 2\|\varphi_2'\|^2_{L^2}$: hence $\lambda_2(\mathcal{G}) = \frac{\|\varphi_2'\|^2_{L^2}}{\|\varphi_2\|^2_{L^2}} \geq \min_{\substack{f \in H^1(\mathcal{G}_{(2)}) \\ f \perp \mathbf{1}_{\mathcal{G}_{(2)}}}} \frac{\|f'\|^2_{L^2}}{\|f\|^2_{L^2}} = \lambda_2(\mathcal{G}_{(2)})$.
- Cut through all vertices to turn $\mathcal{G}_{(2)}$ into a cycle $\mathcal{C}$: this is possible because each vertex in $\mathcal{G}_{(2)}$ has even degree, so $\mathcal{G}_{(2)}$ contains a Eulerian cycle: $\lambda_2(\mathcal{G}_{(2)} \geq \lambda_2(\mathcal{C})$.
- However, $\lambda_2(\mathcal{C}) = \frac{4\pi^2}{|\mathcal{C}|^2} = \frac{\pi^2}{|\mathcal{G}|^2}$.

Selected surgery principles

Proposition (Kennedy–Kurasov–Malenová–M. 2016)

Given $\mathcal{G}$ with finitely many edges of finite length, produce $\mathcal{G}'$ by

1. *cutting through a vertex* v *to create two new vertices* $\mathsf{v}_1, \mathsf{v}_2 \in \mathcal{G}$, *or*
2. *attaching a pendant graph* $\mathcal{H}$ *at a vertex* $\mathsf{v} \in \mathcal{G}$.

Then $\lambda_k(\mathcal{G}) \geq \lambda_k(\mathcal{G}')$.
Furthermore, $\lambda_2(\mathcal{G}) = \lambda_2(\mathcal{C})$ *if*

3. $\mathcal{G}$ *is a figure-8 graph and* $\mathcal{C}$ *is a cycle graph with* $|\mathcal{G}| = |\mathcal{C}|$.

Proof.

(1) $H^1(\mathcal{G}) \supset H^1(\mathcal{G}')$
(2) Take (λ_2, φ_2) and extend φ_2 by continuity to a function that is constant on $\mathcal{H}$. Then $\varphi_2 \mathbf{1}_{\mathcal{G}} - |\mathcal{H}| \mathbf{1}_{\mathcal{H}}$ is orthogonal to $\mathbf{1}_{\mathcal{G}'}$, hence an admissible test function for $\lambda_2(\mathcal{G}')$.
(3) Construct $\mathcal{C}$ from $\mathcal{G}$ by cutting through the (only) vertex v, thus creating $\mathsf{v}_1, \mathsf{v}_2$. By (1), $\lambda_2(\mathcal{C}) \leq \lambda_2(\mathcal{G})$.
Pick a ground state ψ_2 on $\mathcal{C}$: up to rotation, wlog $\psi_2(\mathsf{v}_1) = \psi_2(\mathsf{v}_2)$: thus, $\psi_2 \in H^1(\mathcal{G})$ is an admissible test function on $\mathcal{G}$, hence $\lambda_2(\mathcal{G}) \leq \lambda_2(\mathcal{C})$. □

An upper estimate

Theorem (Kennedy–Kurasov–Malenová–M. 2016)

For any metric graph $\mathcal{G}$ on $E \geq 2$ edges of finite length

$$\lambda_2(\mathcal{G}) \leq \frac{\pi^2 E^2}{|\mathcal{G}|^2}.$$

Equality holds for equilateral stars and equilateral pumpkin graphs...

M.–Pivovarchik 2022: ...and for an infinite class of metric graphs ("inflated stars", after Butler–Grout 2011).

Proof

- Glue *all* vertices to produce a new metric graph $\mathcal{G}'$ (a "metric flower"): then $\lambda_2(\mathcal{G}) \leq \lambda_2(\mathcal{G}')$.
- Produce a figure-8 graph $\mathcal{G}''$ by plucking all petals of the metric flower but the two longest ones: then $\lambda_j(\mathcal{G}') \leq \lambda_j(\mathcal{G}'')$ for all j.
- $\lambda_2(\mathcal{G}'') = \lambda_2(\text{Cycle of same total length as } \mathcal{G}') = \frac{4\pi^2}{|\mathcal{G}''|^2}$ (easy proof using symmetry).
- However, by the pigeonhole principle $|\mathcal{G}''| \geq 2\frac{|\mathcal{G}|}{E}$.

Weyl asymptotics

Recall:

$$\lambda_j(\Delta_{\mathcal{G}}) \geq \frac{\pi^2 (j+1)^2}{4|\mathcal{G}|^2} \qquad \text{for all } j \in \mathbb{N},$$

Proposition

Given $\mathcal{G}$ on $E < \infty$ edges of finite length,

$$\lambda_j(\mathcal{G}) \leq \frac{E^2 \pi^2 (j+1)^2}{|\mathcal{G}|^2}$$

Proof.

Repeat the previous proof and, in the last step, observe that $\lambda_j(\mathcal{G}'') \leq \lambda_{j+1}(\text{Cycle of same total length as } \mathcal{G}') \leq \frac{(j+1)^2 \pi^2}{|\mathcal{G}''|^2}$ (again by symmetry). □

Corollary (Nicaise 1987)

$$\frac{\lambda_j(\mathcal{G})}{j^2} \approx \frac{\pi^2}{|\mathcal{G}|^2}$$

Weyl asymptotics

Recall:

$$\lambda_j(\Delta_{\mathcal{G}}) \geq \frac{\pi^2 (j+1)^2}{4|\mathcal{G}|^2} \qquad \text{for all } j \in \mathbb{N},$$

Proposition

Given $\mathcal{G}$ on $E < \infty$ edges of finite length,

$$\lambda_j(\mathcal{G}) \leq \frac{E^2 \pi^2 (j+1)^2}{|\mathcal{G}|^2}$$

Proof.

Repeat the previous proof and, in the last step, observe that
$\lambda_j(\mathcal{G}'') \leq \lambda_{j+1}(\text{Cycle of same total length as } \mathcal{G}') \leq \frac{(j+1)^2 \pi^2}{|\mathcal{G}''|^2}$ (again by symmetry). □

Corollary (Nicaise 1987)

$$\frac{\lambda_j(\mathcal{G})}{j^2} \approx \frac{\pi^2}{|\mathcal{G}|^2}$$

Eigenvalue estimates with Dirichlet vertex conditions

Proposition (Plümer 2022)

If $\mathcal{G}$ is a graph with finitely many edges of finite length, then

$$\lambda_1(\mathcal{G}; \mathrm{V}^{\mathrm{D}}) \geq \frac{1}{|\mathcal{G}| \operatorname{Inr}(\mathcal{G}; \mathrm{V}^{\mathrm{D}})}$$

where $\operatorname{Inr}(\mathcal{G}; \mathrm{V}^{\mathrm{D}}) := \sup_{x \in \mathcal{G}} d(x, \mathrm{V}^{\mathrm{D}})$.

Proof.

Let $f \in H_0^1(\mathcal{G}; \mathrm{V}^{\mathrm{D}})$, $x \in \mathcal{G}$, $\mathsf{v} \in \mathrm{V}^{\mathrm{D}}$, γ a geodesic between x, v. Then

$$f(x) = f(x) - f(\mathsf{v}) = \int_\gamma f'(y) \,\mathrm{d}y$$

and

$$|f(x)|^2 \leq L(\gamma) \int_\gamma |f'(y)|^2 \,\mathrm{d}y \leq d(x, \mathrm{V}^{\mathrm{D}}) \|f'\|^2_{L^2(\mathcal{G})}.$$

Therefore,

$$\|f\|^2_{L^2(\mathcal{G})} \leq \int_{\mathcal{G}} d(x, \mathrm{V}^{\mathrm{D}}) \,\mathrm{d}x \|f'\|^2_{L^2(\mathcal{G})} = |\mathcal{G}| ⨍_{\mathcal{G}} d(x, \mathrm{V}^{\mathrm{D}}) \,\mathrm{d}x \|f'\|^2_{L^2(\mathcal{G})}$$

$$\leq |\mathcal{G}| \operatorname{Inr}(\mathcal{G}; \mathrm{V}^{\mathrm{D}}) \|f'\|^2_{L^2(\mathcal{G})}.$$

Lower estimate by diameter and nodal counting

Corollary (Plümer 2022)

If $\mathcal{G}$ is a graph with finitely many edges of finite length, then

$$\lambda_2(\mathcal{G}) \geq \frac{2}{|\mathcal{G}| \operatorname{Diam}(\mathcal{G})}.$$

Shape optimization wrt heat kernel?

Recall: If $\mathcal{G}, \mathcal{G}'$ are two different wirings over the same edge set,

$$p_t^{\mathcal{G}}(x,y) \le p_t^{\mathcal{G}'}(x,y) \qquad \forall x,y \in \mathcal{G}$$

for all $t \ge 0$ is impossible.

Alternative idea: Consider the **overall insulation** wrt $\mathrm{V^D}$

$$\int_0^\infty \int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G};\mathrm{V^D}}(x,y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t.$$

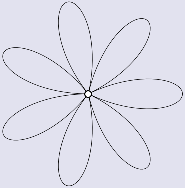
Remark

- Because $p_t^{\mathcal{G}} \ge 0$, so is $\int_0^\infty \int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G}}(x,y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t$.
- The Green function $G^{\mathcal{G};\mathrm{V^D}}$ is the Laplace transform of $p_\cdot^{\mathcal{G};\mathrm{V^D}}$ (Exercise).
- If $\mathrm{V^D} = \emptyset$, the overall insulation is always $= \infty$, because $\int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G};\mathrm{V^D}}(x,y)\,\mathrm{d}x\,\mathrm{d}y = |\mathcal{G}|$ (Exercise).

Path graphs maximize insulation

Theorem

$$\frac{1}{12}\frac{|\mathcal{G}|^3}{\#\mathsf{E}^3} \leq \int_0^\infty \int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G}}(x,y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t \leq \frac{1}{3}|\mathcal{G}|^3$$

Lower estimate is an equality iff $\mathcal{G}=$ 

Upper estimate is an equality iff $\mathcal{G}=$ 

Proof (upper estimate)

- $\int_0^\infty p_t^{\mathcal{G}}(x,y)\,\mathrm{d}t$ is the Green's function of $\mathcal{G}$, i.e., the integral kernel of Δ^{-1}.
- Thus, $\int_0^\infty \int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G}}(x,y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t = -\int_{\mathcal{G}} \Delta^{-1}\mathbb{1}(x)\,\mathrm{d}x$
- Describe the integrated heat content in variational terms, following Pólya:

$$-\int_{\mathcal{G}} (\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}})^{-1}\mathbb{1}(x)\,\mathrm{d}x = \max_{u\in H_0^1(\mathcal{G};\mathrm{V}^\mathrm{D})} \frac{\|u\|_{L^1}^2}{\|u'\|_{L^2}^2}$$

  because the Euler–Lagrange equation for

$$-\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}}\, u = \mathbb{1}$$

  is

$$\frac{1}{2}\int_{\mathcal{G}} u'(x)h'(x)\,\mathrm{d}x = \int_{\mathcal{G}} h(x)\,\mathrm{d}x, \qquad h \in H_0^1(\mathcal{G};\mathrm{V}^\mathrm{D})$$

- Mimic Nicaise' doubling trick.

Proof (lower estimate)

- Use again $\int_0^\infty \int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G}}(x,y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t = \max_{u\in H_0^1(\mathcal{G};\mathsf{V}^{\mathrm{D}})} \frac{\|u\|_{L^1}^2}{\|u'\|_{L^2}^2}$
- Consider, as a test function, the function u^* that satisfies $-{u^*}_{\mathsf{e}}'' = \mathbb{1}$ with Dirichlet conditions on each edge.
- Check that

$$\frac{\|u^*_{\mathsf{e}}\|_{L^1}^2}{\|{u^*}_{\mathsf{e}}'\|_{L^2}^2} = \frac{\#\mathsf{E}^3}{12}$$

and use Jensen.

Landscape functions on metric graphs, after Filoche–Mayboroda

Theorem (M. 2024)

Let $\mathsf{V}^{\mathrm{D}} \neq \emptyset$*. Then each eigenpair* (λ, φ) *of* $-\Delta_{\mathcal{G};\mathsf{V}^{\mathrm{D}}}$ *satisfies*

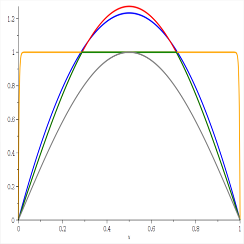
$$\frac{|\varphi(x)|}{\|\varphi\|_\infty} \leq \inf_{\delta>0} \delta \left[\left(-\lambda_1 + \delta - \left((-\Delta_{\mathcal{G};\mathsf{V}^{\mathrm{D}}})^{-1} \mathbb{1} \right) \right] (x)$$

Landscape functions on metric graphs, after Filoche–Mayboroda

Theorem (M. 2024)

Let $\mathrm{V}^{\mathrm{D}} \neq \emptyset$. *Then each eigenpair* (λ, φ) *of* $-\Delta_{\mathcal{G};\mathrm{V}^{\mathrm{D}}}$ *satisfies*

$$\frac{|\varphi(x)|}{\|\varphi\|_\infty} \leq \inf_{\delta>0} \delta \left[\left(-\lambda_1 + \delta - \left((-\Delta_{\mathcal{G};\mathrm{V}^{\mathrm{D}}})^{-1}\mathbb{1}\right)\right] (x)$$



Application to the heat kernel of Laplacians $\Delta_{\mathcal{G};\mathrm{V}^{\mathrm{D}}}$

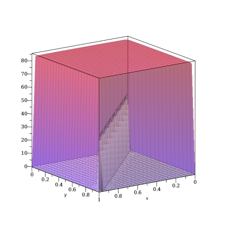
Proposition

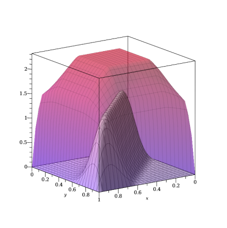
There exists $C = C(\mathcal{G})$ *with*

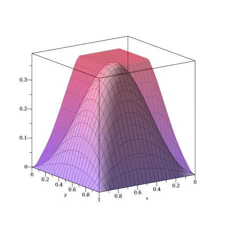
$$p_t^{\mathcal{G};\mathrm{V}^{\mathrm{D}}}(x,y) \le C \left[\sum_{k\in\mathbb{N}} |\lambda_k|^2 \mathrm{e}^{-t\lambda_k} \right] (-\Delta_{\mathcal{G};\mathrm{V}^{\mathrm{D}}})^{-1}\mathbb{1}(x)(-\Delta_{\mathcal{G};\mathrm{V}^{\mathrm{D}}})^{-1}\mathbb{1}(y).$$

Example

Simplest case: $\mathcal{G}$ = interval $(0,1)$ with Dirichlet conditions at both endpoints







Same estimates holds even for the heat kernel of the magnetic Laplacian!

Proof

- Consider an ONB of eigenvectors of $\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}}$. Then

$$\varphi_k = \lambda_k(\Delta_\alpha^{\mathcal{G};\mathrm{V}^\mathrm{D}})^{-1}\varphi_k$$

and because $\mathrm{e}^{t\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}}}$ is positive

$$|\varphi_k| = |(\Delta_\alpha^{\mathcal{G};\mathrm{V}^\mathrm{D}})^{-1}\varphi_k| \leq |\lambda_k|(-\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}})^{-1}|\varphi_k| \leq |\lambda_k|\|\varphi_k\|_\infty(-\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}})^{-1}\mathbb{1}.$$

- Bifulco–Kerner 2024: $\rightsquigarrow$ $\|\varphi_k\|_\infty \leq C(\mathcal{G})$ for some $C = C(\mathcal{G})$ and all k.
- Mercer Theorem $\rightsquigarrow$

$$\begin{aligned}|p_t^{\mathcal{G};\mathrm{V}^\mathrm{D}}(x,y)| &= \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k(\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}})}|\varphi_k(x)|\,|\varphi_k(y)| \\ &\leq C(\mathcal{G})^2 \sum_{k\in\mathbb{N}} |\lambda_k|^2 \mathrm{e}^{-t\lambda_k}(-\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}})^{-1}\mathbb{1}(x)(-\Delta_{\mathcal{G};\mathrm{V}^\mathrm{D}})^{-1}\mathbb{1}(y).\end{aligned}$$

Torsion function can be computed explicitly

Exercise

Let $\mathcal{G}$ be equilateral ($\ell_{\mathsf{e}} \equiv 1$) and let $v := (-\Delta_{\mathcal{G};\mathsf{V}^{\mathrm{D}}})^{-1}\mathbb{1}$, for $\mathsf{V}^{\mathrm{D}} \neq \emptyset$. Then the restriction $g := v_{|\mathsf{V}} : \mathsf{V} \to \mathbb{R}$ is the unique solution of the system

$$\begin{cases} g(\mathsf{v}) = 0, & \mathsf{v} \in \mathsf{V}^{\mathrm{D}}, \\ \dfrac{1}{\deg(\mathsf{v})} \displaystyle\sum_{\mathsf{w} \sim \mathsf{v}} g(\mathsf{v}) - g(\mathsf{w}) = \dfrac{1}{2}, & \mathsf{v} \in \mathsf{V} \setminus \mathsf{V}^{\mathrm{D}}. \end{cases}$$

References

- Kramar–Fijavž–M.–Sikolya, *Variational and semigroup methods for waves and diffusion on networks*, AMO 2007
- M.–Romanelli, *Dynamic and generalized Wentzell node conditions for network equations*, MMAS 2007
- Kennedy–Kurasov–Malenová–M., *On the spectral gap of a quantum graph*, Ann. Poincaré 2016
- Berkolaiko–Kennedy–Kurasov–M., *Edge connectivity and the spectral gap of combinatorial and quantum graphs*, J. Phys. A 2017
- Hussein–M., *Laplacians with point interactions – expected and unexpected spectral properties*, in: Semigroups of Operators – Theory and Applications, Springer 2020.
- Glück–M., *Eventual Domination for Linear Evolution Equations*, Math. Z. 2021
- Hofmann–Kennedy–M.–Plümer, *On Pleijel's nodal domain theorem for quantum graphs*, Ann. H. Poincaré 2021
- M.–Plümer, *On torsional rigidity and ground-state energy of compact quantum graphs*, Calc. Var. 2023
- Bifulco–M., *On the Lipschitz continuity of the heat kernel*, arXiv:2307.08889
- Bifulco–M., *On the heat content of compact quantum graphs*, arXiv:2502.09461

Commercial #1

COST (`cost.eu`) just approved the Action
multiscale Stochastics, Patterns, and Analysis
of Combinatorial Environments (mSPACE).

- 40 applicants from 20 European countries
- Financial support for Short Term Scientific Missions
- . . . and the organisation of summer schools
- . . . and of conferences, workshops, minisymposia, special sessions, . . .

- Participation open to new members, too. . .
- . . . from countries in North Africa and Middle East (and Europe)
- Applications open from June 12, 2025
- Please reach out if interested!

Commercial #2

African–European Early-Career

Network of Female Mathematicians

in Mathematical Physics and Analysis

- Interest in taking parts in online (to begin with...) mathematical meetings with fellow female mathematicians from Africa and Europe?
- Then reach out: Anna Liza Schonlau (University of Bonn) schonlau@iam.uni-bonn.de

Thank you for your attention!