

# Surgery of quantum graphs: eigenvalues and heat kernels

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March 22, 2018

# Über ein Paradoxon aus der Verkehrsplanung

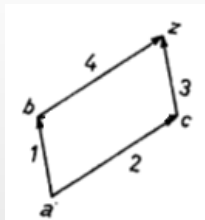
Von D. BRAESS, Münster<sup>1)</sup>

Eingegangen am 28. März 1968

*Zusammenfassung:* Für die Straßenverkehrsplanung möchte man den Verkehrsfluß auf den einzelnen Straßen des Netzes abschätzen, wenn die Zahl der Fahrzeuge bekannt ist, die zwischen den einzelnen Punkten des Straßennetzes verkehren. Welche Wege am günstigsten sind, hängt nun nicht nur von der Beschaffenheit der Straße ab, sondern auch von der Verkehrsdichte. Es ergeben sich nicht immer optimale Fahrzeiten, wenn jeder Fahrer nur für sich den günstigsten Weg herausucht. In einigen Fällen kann sich durch Erweiterung des Netzes der Verkehrsfluß sogar so umlagern, daß größere Fahrzeiten erforderlich werden.

*Summary:* For each point of a road network let be given the number of cars starting from it, and the destination of the cars. Under these conditions one wishes to estimate the distribution of the traffic flow. Whether a street is preferable to another one depends not only upon the quality of the road but also upon the density of the flow. If every driver takes that path which looks most favorable to him, the resultant running times need not be minimal. Furthermore it is indicated by an example that an extension of the road network may cause a redistribution of the traffic which results in longer individual running times.

# Braess' paradox



In diesem Zusammenhang erkennt man auch eine paradoxe Tatsache. Wenn in dem Netz des Modellbeispiels der Bogen  $u_5$  eliminiert wird, fällt der kritische Fluß mit dem optimalen zusammen; der Fluß wird dann also besser verteilt. Für die Verkehrspraxis bedeutet das: In ungünstigen Fällen kann durch eine Erweiterung des Straßennetzes der Zeitaufwand anwachsen.

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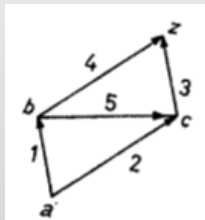


Figure: D. Braess 1968

**Networks don't necessarily become more efficient by merely getting denser and denser!**

In the context of quantum graphs:

- ▶ Exner-Jex 2012
- ▶ Kurasov-Malenová-Naboko 2013

# Outline

- ▶ Discrete graphs
- ▶ Quantum graphs
- ▶ Heat kernels

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Discrete  
Laplacians

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Spectral  
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Let  $G = (V, E)$  be a loopless (finite) graph (possibly a multigraph, no loops!).

Regard  $f : V \rightarrow \mathbb{C}$  as a function on  $G$ : the natural Hilbert space is  $\ell^2(V) \simeq \mathbb{C}^V$ .

Upon choosing an arbitrary orientation, consider the incidence matrix  $\mathcal{I} = (\iota_{ve})$ :

$$\iota_{ve} := \begin{cases} -1 & \text{if } v \text{ is initial endpoint of } e, \\ +1 & \text{if } v \text{ is terminal endpoint of } e, \\ 0 & \text{otherwise} \end{cases}$$

Then

$$\mathcal{L}^G := \mathcal{I}\mathcal{I}^T$$

defines a (bounded) self-adjoint, positive semidefinite operator on  $\ell^2(V)$ : the *discrete Laplacian* (Kirchhoff 1847, Brooks-Smith-Stone-Tutte 1940, Anderson-Morley 1971).

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# Spectral graph theory

The spectrum  $\{0 = \lambda_0, \lambda_1, \dots, \lambda_{|V|-1}\}$  of  $\mathcal{L}^G$  carries much interesting information:

- ▶ multiplicity of 0 in  $\sigma(\mathcal{L}^G) = \#$  of connected components of  $G$
- ▶ the higher the spectral gap

$$\lambda_1(\mathcal{L}^G) = \inf_{\substack{f \in \ell^2(V) \\ f \perp \mathbf{1}}} \frac{\|\mathcal{I}^T f\|_{\ell^2(E)}^2}{\|f\|_{\ell^2(V)}^2}$$

the more connected  $G$  ( $\lambda_1(\mathcal{L}^G)$  is also called *algebraic connectivity* of  $G$ ).

- ▶ Eigenfunctions associated with  $\lambda_1(\mathcal{L}^G), \lambda_2(\mathcal{L}^G)$  induce *very reasonable* drawings of planar graphs
- ▶ ... (see e.g. Spielman 2007, Spielman 2010)

# “Qualitative” spectral graph theory

**Idea:** relate spectral quantities of  $\mathcal{L}^G$  with some combinatorial quantities of  $G$ .

## Example

- ▶ *Fiedler 1973:*  $\eta \geq \lambda_1(\mathcal{L}^G) \geq 2\eta \left(1 - \cos \frac{\pi}{|V|}\right)$
- ▶ *Dodziuk 1984, Alon-Milman 1985:*  
 $2h \geq \lambda_1(\mathcal{L}^G) \geq \frac{h^2}{2 \deg_{\max}}$
- ▶ *McKay 1988, Chung 1989, Mohar 1991:*  
 $\frac{\deg_{\max}(|V|-1)}{(2D-|V|+1)_+} \geq \lambda_1(\mathcal{L}^G) \geq \frac{4}{|V|D}$

( $\eta$  edge connectivity,  $h$  Cheeger constant of  $G$ ,  
 $\deg_{\max}$  maximal degree,  $D$  diameter)

Inserting edges *tends* to lower  $\lambda_1(\mathcal{L}^G)$ , but...

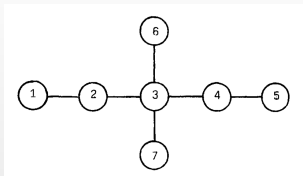
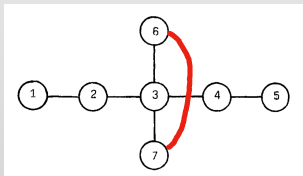


Figure: C. Maas 1987

... sometimes  $\lambda_1(\mathcal{L}^G) = \lambda_1(\mathcal{L}^{G'})$



# Quantum graphs

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A *quantum graph* (or *metric graph*, or *network*)  $\mathcal{G}$  is obtained by associating an interval  $(0, \ell_e)$  of length  $\ell_e$  with each edge  $e$  of  $G = (V, E)$ .

Natural Hilbert space on  $\mathcal{G}$ :

$$L^2(\mathcal{G}) := \bigoplus_{e \in E} L^2(0, \ell_e)$$

No boundary conditions can be imposed on functions in  $L^2(\mathcal{G})$ , so **functions in  $L^2(\mathcal{G})$  do not see the combinatorics of  $\mathcal{G}$ .**

Introduce

$$C(\mathcal{G}) := \left\{ f \in \bigoplus_{e \in E} C[0, \ell_e] : f \text{ is continuous in each } v \in V \right\}$$

and

$$H^1(\mathcal{G}) := \left\{ f = (f_e)_{e \in E} \in C(\mathcal{G}) : f_e \in H^1(0, \ell_e) \quad \forall e \in E \right\}$$

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# Spectral gap of quantum graphs

In analogy with

$$\lambda_1(\mathcal{L}^G) = \inf_{\substack{f \in \ell^2(\mathbf{V}) \\ f \perp 1}} \frac{\|\mathcal{I}^T f\|_{\ell^2(\mathbf{E})}^2}{\|f\|_{\ell^2(\mathbf{V})}^2} \quad \text{and} \quad \lambda_1(\Delta) = \inf_{\substack{f \in H^1(0,1) \\ f \perp 1}} \frac{\|f'\|_{L^2(0,1)}^2}{\|f\|_{L^2(0,1)}^2}$$

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consider

$$\lambda_1(\Delta_G) := \inf_{\substack{f \in H^1(\mathcal{G}) \\ f \perp 1}} \frac{\|f'\|_{L^2(\mathcal{G})}^2}{\|f\|_{L^2(\mathcal{G})}^2}$$

$\lambda_1(\Delta_G)$  is the spectral gap of  $\Delta_G$ , the self-adjoint, positive semidefinite operator on  $L^2(\mathcal{G})$  associated with

$$a(f) := \sum_{e \in E} \int_0^{\ell_e} |f'|^2, \quad f \in H^1(\mathcal{G})$$

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consider

$$\lambda_1(\Delta_{\mathcal{G}}) := \inf_{\substack{f \in H^1(\mathcal{G}) \\ f \perp 1}} \frac{\|f'\|_{L^2(\mathcal{G})}^2}{\|f\|_{L^2(\mathcal{G})}^2}$$

$\lambda_1(\Delta_{\mathcal{G}})$  is the spectral gap of  $\Delta_{\mathcal{G}}$ , the self-adjoint, positive semidefinite operator on  $L^2(\mathcal{G})$  associated with

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A secular equation yielding all eigenvalues of  $\Delta_{\mathcal{G}}$  is known (von Below 1985, Kottos-Smilansky 1997) but is useless in practice.

# Spectral estimates for quantum graphs

## Proposition (Nicaise 1987)

- ▶  $\lambda_1(\Delta_{\mathcal{G}}) \geq \frac{\pi^2}{L^2}$
- ▶  $\lambda_1(\Delta_{\mathcal{G}}) \geq \frac{h^2}{4}$

Nicaise' first estimate is sharp: it is attained for path graphs.

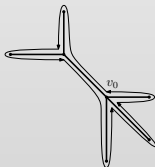
Also the second estimate can be shown to be sharp, adapting an example invented by Buser.

( $L$  total length,  $h$  Cheeger constant of  $\mathcal{G}$ )

(Many *upper* estimates by Kennedy-Kurasov-Malenová-M. 2016; Band-Lévy 2016; Rohleder 2016; Aritürk 2016)

# Proof of Nicaise' isoperimetric inequality #1

- ▶ Cut through all cycles of  $\mathcal{G}$  to turn it into a tree  $\mathcal{G}'$ : since  $H^1(\mathcal{G}) \subset H^1(\mathcal{G}')$ , this lowers the Rayleigh quotient.
- ▶ Consider the double cover  $\mathcal{G}'_{(2)}$  of the tree  $\mathcal{G}'$  (i.e., double each edge): the total length is  $2L$ .
- ▶ Each  $f \in H^1(\mathcal{G})$  induces  $f_{(2)} \in H^1(\mathcal{G}'_{(2)})$  canonically: their Rayleigh quotients coincide.
- ▶ For  $f_{(2)} \in H^1(\mathcal{G}'_{(2)})$  define  $g \in H^1(\mathcal{G}'')$  ( $\equiv$  cycle of length  $2L$ ) by suitably dropping a few continuity conditions in the vertices (transverse the graph like in a Eulerian cycle).



$\Rightarrow H^1(\mathcal{G}'_{(2)})$  can be naturally embedded in  $H^1(\mathcal{G}'')$

# Proof of Nicaise' isoperimetric inequality #2

- ▶ If  $f$  is an eigenfunction for  $\lambda_1(\Delta_{\mathcal{G}})$ ,  $g$  is still a test function for  $\mathcal{G}'' \Rightarrow \lambda_1(\Delta_{\mathcal{G}''})$  is a lower bound for  $\lambda_1(\Delta_{\mathcal{G}})$
- ▶  $\lambda_1(\Delta_{\mathcal{G}''})$  is just the spectral gap (=lowest nonzero eigenvalue) of the second derivative on  $(0, 2L)$  with periodic boundary conditions, i.e.  $\frac{4\pi^2}{(2L)^2}$ .

Nicaise' isoperimetric inequality has been rediscovered/reproved by

- ▶ Solomyak (2002)
- ▶ Friedlander (2005)
- ▶ Berkolaiko-Kennedy-Kurasov-M. (2017)
- ▶ Berkolaiko-Kennedy-Kurasov-M. (2018)

Proposition (Kurasov-Naboko 2014, Band-Lévy 2016)

*Nicaise isoperimetric inequality can be improved to*

$$\lambda_1(\Delta_{\mathcal{G}}) \geq \frac{4\pi^2}{L^2}$$

- ▶ *if  $\mathcal{G}$  is Eulerian;*
- ▶ *if, more generally,  $\mathcal{G}$  is doubly edge connected.*

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Kennedy–Kurasov–Malenová–M. 2016,  
Kennedy–M. 2016,  
Berkolaiko–Kennedy–Kurasov–M. 2017

estimates on $\lambda_1(\Delta_{\mathcal{G}})$	upper	lower
total length	<b>X</b>	$\frac{\pi^2}{L^2}$
total length + # edges	$\frac{\pi^2 E^2}{L^2}$	<b>X</b>
diameter + # vertices	$\frac{\pi^2 (V+1)^2}{D^2}$	<b>X</b>
diameter + # edges	$\frac{4\pi^2 E^2}{D^2}$	$\frac{\pi^2}{D^2 E^2}$
diameter + total length	$\frac{\pi^2 (4L-3D)}{D^3}$	$\frac{1}{DL}$
Cheeger constant	$\frac{\pi^2 h^2 E^2}{4}$	$\frac{h^2}{4}$
edge connectivity + total length	<b>X</b>	$\left( \frac{\eta\pi}{L+\ell_{\max}(\eta-2)^+} \right)^2$



Proposition (Nicaise 1987;  
Berkolaiko-Kennedy-Kurasov-M 2017)

- ▶  $\lambda_0(\Delta_{\mathcal{G}}) \geq \frac{\pi^2}{4L^2}$  if there are Dirichlet vertices.
- ▶  $\lambda_0(\Delta_{\mathcal{G}}) \geq \frac{\pi^2}{D^2}$  if  $\mathcal{G}$  is a tree and all leaves are Dirichlet.
- ▶  $\lambda_0(\Delta_{\mathcal{G}}) \geq \frac{\pi^2}{L^2}$  if there are Dirichlet vertices and the graph is doubly connected.

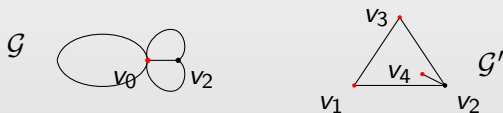
# Surgery of quantum graphs - #1

Proposition (Berkolaiko-Kennedy-Kurasov-M)

$$\lambda_k(\Delta^{\mathcal{G}}) \geq \lambda_k(\Delta^{\mathcal{G}'}) \quad \text{for all } k$$

if  $\mathcal{G}'$  is obtained from  $\mathcal{G}$  by

- ▶ cutting through two previously identified vertices;



- ▶ attaching a pendant (e.g., an edge) to one vertex;
- ▶ lengthening an edge
- ▶ replacing  $k$  parallel edges by one edge of same total length ("unfolding  $\mathcal{G}$ ")



# Surgery of quantum graphs - #2

## Proposition (Berkolaiko-Kennedy-Kurasov-M)

Given any eigenfunction  $\psi$  for  $\lambda_1(\Delta^{\mathcal{G}})$ , then

$$\lambda_1(\Delta^{\mathcal{G}}) \geq \lambda_1(\mathcal{G}')$$

if  $\mathcal{G}'$  is obtained from  $\mathcal{G}$  by

- ▶ deleting an edge where  $\psi$  vanishes identically;
- ▶ inserting an edge of length  $\geq \frac{\pi}{\sqrt{\lambda_1(\Delta^{\mathcal{G}})}}$  between any  $v, w$ ;
- ▶ inserting an edge between any  $v, w$  s.t.  $\psi(v) = \psi(w)$ ;
- ▶ replacing  $k$  parallel edges (along which  $\psi$  is growing) by  $m \leq k$  equilateral edges of same total length;



cutting a subgraph  $\mathcal{H}$  with  $\psi(\mathcal{H}) \subset [0, \kappa]$  and attaching any graph of same length at vertices  $v, w$  with  $\psi(v) = \psi(w)$

# Surgery of quantum graphs - #2

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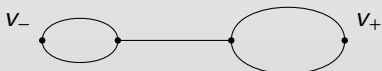
# Comparison principles for quantum graphs

## Proposition (Berkolaiko-Kennedy-Kurasov-M 2017)

- ▶ The lasso graph with loop length  $S$  has lowest  $\lambda_1(\Delta^{\mathcal{G}})$  among all graphs with circumference  $S$ .



- ▶ The dumbbell graph with handle length  $D$  and loops length  $(L - D)/2$  has lowest  $\lambda_1(\Delta^{\mathcal{G}})$  among all graphs with total length  $L$  and diameter  $D$ .



- ▶ The dumbbell graph with handle length  $L - V$  and loops length  $V/2$  has lowest  $\lambda_1(\Delta^{\mathcal{G}})$  among all graphs with doubly connected part of length  $V$ .

# Diffusion on graphs and quantum graphs

Laplacians on graphs and quantum graphs are associated with Dirichlet forms:

- ▶ Beurling-Deny 1959, Keller-Lenz 2010 (discrete graphs)
- ▶ Kramar Fijavž-M-Sikolya 2007 (quantum graphs)

$\Rightarrow e^{-t\mathcal{L}^G}$  and  $e^{t\Delta^G}$  are submarkovian semigroups.

# Parabolic Braess' paradox

Because

$$\sup_{\|f\|_{L^2}=1} \|e^{-t\Delta^{\mathcal{G}}} f - \int_{\mathcal{G}} f\|_{L^2} = o(e^{-t\lambda_1(\Delta^{\mathcal{G}})})$$

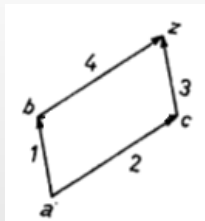
surgery principle can be interpreted for (connected) quantum graphs: e.g.

- ▶ By identifying vertices of a quantum graph, convergence to equilibrium becomes *faster*.
- ▶ If there exist two vertices  $v, w$  and an eigenfunction  $\psi$  (on  $\mathcal{G}$ ) for  $\lambda_1$  s.t.  $\psi(v) = \psi(w)$ , then diffusion on  $\mathcal{G}' := \mathcal{G} \cup vw$  converges to equilibrium *more slowly* than on  $\mathcal{G}$ .

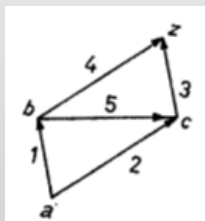
(For comparison: diffusion on  $G' := G \cup vw$  converges to equilibrium *more quickly* than on  $G$ .)

# What about diffusion between pairs of vertices?

Diffusing from  $a$  to  $z$  is faster on



Diffusing from  $b$  to  $c$  is faster on





# Domination: the right notion?

*Domination* of a semigroup  $(e^{tA})_{t \geq 0}$  by another positive semigroup  $(e^{tB})_{t \geq 0}$  means that

$$|e^{tA}f| \leq e^{tB}|f| \quad \text{for all } t \geq 0 \text{ and all } f \geq 0;$$

Examples:

- ▶  $(e^{t\Delta^N})_{t \geq 0}$  dominates  $(e^{t\Delta^D})_{t \geq 0}$ ;
- ▶  $(e^{-t(\Delta^N)^2})_{t \geq 0}$  does *not* dominate  $(e^{t\Delta^N})_{t \geq 0}$ ;

## Proposition (Ouhabaz 1996)

Let  $a \sim A$ ,  $b \sim B$  be Dirichlet forms on  $H$ ,  $D(a) \subset D(b)$ .

TFAE:

- ▶  $e^{tA} \leq e^{tB}$ ;
- ▶  $\operatorname{Re} a(u, v) \geq b(|u|, |v|)$  for all  $u \in D(a)$  and  $v \in D(b)$  such that  $|v| \leq |u|$ ; and additionally,  $D(a)$  is an ideal of  $D(b)$ .

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## Proposition

- ▶ If  $G$  is subgraph of  $G'$ , then  $e^{-t\mathcal{L}^G} \not\leq e^{-t\mathcal{L}^{G'}} \not\leq e^{-t\mathcal{L}^G}$
- ▶ If  $\mathcal{G}'$  is obtained from  $\mathcal{G}$  by cutting through two previously identified vertices, then  $e^{-t\mathcal{L}^{\mathcal{G}}} \not\leq e^{-t\mathcal{L}^{\mathcal{G}'}} \not\leq e^{-t\mathcal{L}^{\mathcal{G}}}$ .

In particular, there is no domination (in either direction) for diffusion on spanning (either combinatorial or quantum) trees.

# Interwoven semigroups

Given  $f > 0$ ,  $(e^{tA}f)_{t \in [0, \infty)}$ ,  $(e^{tB}f)_{t \in [0, \infty)}$  are *interwoven* if for all  $t \in [0, \infty)$  and some  $t_1, t_2 \geq t$  one has

$$e^{t_1 B} f > e^{t_1 A} f \quad \text{and} \quad e^{t_2 A} f > e^{t_2 B} f.$$

Theorem (Glück-M 2018)

Let  $(X, \mu)$  be a finite measure space and  $A, B$  be **distinct** self-adjoint operators on  $L^2(X, \mu)$ . If  $(e^{tA})_{t \geq 0}, (e^{tB})_{t \geq 0}$  are positive and map  $L^2(X)$  into  $L^\infty(X)$ , then TFAE:

- $s(A) = s(B)$
- there exists  $0 < f \in L^2$  such that the orbits  $(e^{tA}f)_{t \geq 0}$  and  $(e^{tB}f)_{t \geq 0}$  are interwoven.

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Let  $(X, \mu)$  be a finite measure space and  $A, B$  be **distinct** self-adjoint operators on  $L^2(X, \mu)$ . If  $(e^{tA})_{t \geq 0}, (e^{tB})_{t \geq 0}$  are positive and map  $L^2(X)$  into  $L^\infty(X)$ , then TFAE:

- ▶  $s(A) = s(B)$
- ▶ there exists  $0 < f \in L^2$  such that the orbits  $(e^{tA}f)_{t \geq 0}$  and  $(e^{tB}f)_{t \geq 0}$  are interwoven.

## Proposition

- ▶ If  $G, G'$  are two graphs on  $V$ , then there exists  $0 < f \in \ell^2(V)$  such that  $(e^{-t\mathcal{L}^G} f)_{t \geq 0}$  and  $(e^{-t\mathcal{L}^{G'}} f)_{t \geq 0}$  are interwoven.
- ▶ If  $\mathcal{G}, \mathcal{G}'$  are two quantum graphs of same total length, then there exists  $0 < u \in L^2(\mathcal{G})$  such that  $(e^{-t\Delta^{\mathcal{G}}} u)_{t \geq 0}$  and  $(e^{-t\Delta^{\mathcal{G}'}} u)_{t \geq 0}$  are interwoven.

**Thank you for your attention!**