## Quantum Graphs which Optimize the Spectral Gap



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Joint work with Guillaume Lévy, Université Pierre et Marie Curie, Paris (arXiv:1608.00520)

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## Eigenvalue optimization problems (for domains)

Fixing the topology, total volume and boundary conditions, we seek for the shape which maximizes $\backslash$ minimizes an eigenvalue.

## Simply connected domains

Faber-Krahn [Dirichlet conditions]: the ball minimizes $\lambda_{1}$ (no sense maximizing). Krahn-Szegö [Dirichlet conditions]: No minimizer for $\lambda_{2}$, but union of two balls serves as an infimizer.

Szegö-Weinberger [Neumann conditions]: the ball maximizes $\lambda_{1}$ (no sense minimizing).

Multi connected domains
Payne-Weinberger: Planar domains with a single hole,
Dirichlet on outer boundary and Neumann on inner.
Fixing total area and length of outer boundary - annulus (concentric circles) maximizes $\lambda_{1}$

More works by: Ashbaugh-Chatelain, Ashbaugh-Benguria, Exner-Mantile, Flucher,
Harrell-Kröger-Kurata Hersch Kolokolnikov-Titcombe-Ward and more...

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# Outline 

## Introduction

Infimizers

Supremizers
Upper bounds
Spectral gap as a simple eigenvalue
Gluing graphs

Summary \& Conjectures

## From a Discrete graph to a Quantum graph

$\mathcal{G}$ a discrete graph with $E<\infty$ edges and $V<\infty$ vertices. Space of edge lengths:
$\mathscr{L}_{\mathcal{G}}:=\left\{\left(I_{1}, \ldots, I_{E}\right) \in \mathbb{R}^{E} \mid \sum_{e=1}^{E} I_{e}=1\right.$ and $\left.\forall e, I_{e}>0\right\}$
$\Gamma(\mathcal{G} ; \underline{I})$ denotes the metric graph obtained from $\mathcal{G}$ with edge lengths $\underline{I} \in \mathscr{L}_{\mathcal{G}}$.
Namely, the $e^{\text {th }}$ edge corresponds to an interval $\left[0, l_{e}\right]$
Consider the following eigenvalue equation on each $\left[0, l_{e}\right]: \quad-\left.\frac{d^{2}}{d x_{e}^{2}} f\right|_{e}=\left.k^{2} f\right|_{e}$
with the Neumann (Kirchhoff) vertex conditions:


The spectrum, $\left\{k_{n}^{2}\right\}_{n=1}^{\infty}$ is discrete and bounded from below: $0=k_{0}<k_{1} \leq k_{2} \leq$

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Continuity $\quad \forall e_{1}, e_{2} \sim v ;\left.f\right|_{e_{1}}(v)=\left.f\right|_{e_{2}}(v)$
Vanishing sum of derivatives $\left.\sum_{e \sim v} \frac{d}{d x_{e}} f\right|_{e}(v)=0$
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$$
0=k_{0}<k_{1} \leq k_{2} \leq \ldots
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We call $\boldsymbol{k}_{\mathbf{1}}$ the spectral gap of the graph.

Spectral gap dependence on edge lengths
$\mathscr{L}_{g}:=\left\{\left(l_{1}, \ldots, I_{E}\right) \in \mathbb{R}^{E} \mid \sum_{e=1}^{E} l_{e}=1\right.$ and $\left.\forall e, l_{e}>0\right\}$.
$\Gamma(\mathcal{G} ; \underline{I})$ denotes the metric graph obtained from $\mathcal{G}$ with edge lengths $\underline{I} \in \mathscr{L}_{\mathcal{G}}$. Spectral gap is denoted $k_{1}[\Gamma(\mathcal{G} ; \underline{I})] . \quad$ Note: $k_{1}[\Gamma(\mathcal{G} ; \underline{I})]$ is continuous in $\underline{I}$, which leads to consider also $\underline{I} \in \partial \mathscr{L}_{\mathcal{G}}$ (some edge lengths vanish), possibly changing the topology of $\Gamma(\mathcal{G} ; I)$.

Definition 1.


- $\Gamma\left(\mathcal{G} ; \underline{I}^{*}\right)$ a supremizer of $\mathcal{G}$ if $\underline{I}^{*} \in \overline{\mathscr{L}}_{\mathcal{G}}$ and $k_{1}\left[\Gamma\left(\mathcal{G} ; \underline{I}^{*}\right)\right] \geq k_{1}[\Gamma(\mathcal{G} ; I)], \forall \underline{I} \in \overline{\mathscr{L}}_{\mathcal{G}}$.
- Same definitions for minimizer and infimizer.
- Supremizer and infimizer always exist

What about maximizer minimizer?


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- Which graphs are spectral gap optimizers?



## Quantum Graphs which Optimize the Spectral Gap

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A few examples

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\begin{aligned}
& \text { Star graph with } E \geq 2 \text { edges } \\
& \text { Infimum (no minimum): } k_{1}(1,0, \ldots 0)=\pi \\
& \text { Maximum: } k_{1}(1 / E, \ldots, 1 / E)=\frac{E}{2} \pi \quad \text { (equilateral star) } \\
& \text { (Recall: total edge length }=1 \text { ) }
\end{aligned}
$$

Flower graph with $E \geq 2$ edges
Infimum (no minimum): $k_{1}(1,0, \ldots 0)=2 \pi$,
Maximum: $k_{1}(1 / E, \ldots, 1 / E)=E \pi \quad$ (equilateral flower)
[Kennedy, Kurasov, Malenová, Mugnolo '16]

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$k_{1}\left(l_{1}, l_{2}, l_{3}\right)$

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## Quantum Graphs which Optimize the Spectral Gap

A few examples (continued)


Stowe (Flétoile) graph with $E_{p}$ petals, $E_{l}$ leaves
Infimum (no minimum): $k_{1}(0 \ldots, 0,1)=\pi$,
Maximum: $k_{1}(\underline{I})=\left(E_{p}+\frac{E_{l}}{2}\right) \pi$,
where $\underline{I}=\frac{1}{2 E_{p}+E_{l}}(\underbrace{2, \ldots, 2}_{E_{p}}, \underbrace{1, \ldots, 1}_{E_{I}})$ ("equilateral" shower),
assuming $E_{p}+E_{l} \geq 2$ and $\left(E_{p}, E_{l}\right) \notin(1,1)$. [Shown in future slide].
This generales stars and flowers results.

## Quantum Graphs which Optimize the Spectral Gap

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Infimum: $k_{1}(0,0,1)=\pi$,
Maximum: $k_{1}\left(\frac{2}{5}, \frac{2}{5}, \frac{1}{5}\right)=2 \frac{1}{2} \pi$

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\begin{aligned}
& E_{p}=1 \\
& E_{I}=2
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Infimum: $k_{1}(0,0,1)=\pi$,
Maximum: $k_{1}\left(\frac{2}{5}, \frac{2}{5}, \frac{1}{5}\right)=2 \frac{1}{2} \pi$
Continuous family of infima: $k_{1}(0, t, 1-t)=\pi$, Continuous family of maxima: $k_{1}(1-2 t, t, t)=2 \pi$

## Quantum Graphs which Optimize the Spectral Gap

A few examples (continued)


Mandarin graph with $E$ edges
Infimum (no minimum): $k_{1}(1,0, \ldots, 0)=2 \pi$, Maximum: $k_{1}(1 / E, \ldots, 1 / E)=E \pi$.
[Kennedy, Kurasov, Malenová, Mugnolo '16]

Length dependence figures - courtesy of Lior Alon

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- Which graphs have not only supremizer $\backslash$ infimizer, but also maximizer $\backslash$ minimizer?
- Which graphs are spectral gap optimizers?


# Lower bounds - Known results 

$$
k_{1}[\Gamma] \geq \pi
$$

with equality iff $\Gamma$ is a single edge [Nicaise '87; Friedlander '05; Kurasov, Naboko '14].

If $\Gamma$ has all vertex degrees even then

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k_{1}[\Gamma] \geq 2 \pi, \quad[\text { Kurasov, Naboko '14] }
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with a single loop achieving equality (for example).

Remaining questions:

- What about other topologies?
- What are all possible minimizers \infimizers?


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## Infimizers - Solution

A bridge is an edge whose removal dissconnects the graph.

1. Let $\mathcal{G}$ be a graph with a bridge. Then
1.1 The infimal spectral gap of $\mathcal{G}$ equals $\pi$.
1.2 The unique infimizer is the unit interval.
2. Let $\mathcal{G}$ be a bridgeless graph. Then
2.1 The infimal spectral gap of $\mathcal{G}$ equals $2 \pi$.
2.2 Any infimizer is a symmetric necklace graph.

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## Theorem 2 (Band, Lévy).

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- When is there a minimum?


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- When is there a minimum?
- Proof idea - rearrangment method on graphs.


Figure: symmetric necklace graph

## Upper bounds - Known results

- Global bound

$$
k_{1}[\Gamma] \leq E \pi,
$$

equality if and only if $\Gamma$ is an equilateral mandarin or equilateral flower [Kennedy, Kurasov, Malenová, Mugnolo '16].

This fully answers optimization for flowers and mandarins: supremizers (also maximizers) are equilateral.

- If $\Gamma$ is a tree then

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k_{1}[\Gamma] \leq \frac{E}{2} \pi,
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This fully answers optimization for trees: supremizers are stars.

## Upper bounds - Further progress

## Proposition 3 (Band, Lévy).

If $\Gamma$ is a tree with $E_{l}$ leaves then $k_{1}[\Gamma] \leq \frac{E_{l}}{2} \pi$.

## Proof idea.

$d(\Gamma):=\max \{d(x, y) \mid x, y \in \Gamma\}$ graph diameter.
Combine $k_{1}[\Gamma] \leq \frac{\pi}{d(\Gamma)}$ with $d(\Gamma) \geq \frac{2}{E_{1}}$ (the latter true for trees).

Proposition 4 (Band, Lévy).
Let G be a graph with E edges, out of which El are leaves.
If $\left(E, E_{l}\right) \notin\{(1,1),(1,0),(2,1)\}$ then $\forall \underline{I} \in \mathscr{L}_{\mathcal{G}}, \quad k_{1}[\Gamma(\mathcal{G} ; \underline{l})] \leq \pi\left(E-\frac{E_{l}}{2}\right)$
Assuming $\left(E, E_{l}\right) \notin\{(2,0),(3,2)\}$ equality above implies $\Gamma(\mathcal{G} ; I)$ is
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Take $\Gamma$ and attach two vertices to obtain $\Gamma^{\prime}$ (illegal move in our game). Get $k_{1}(\Gamma) \leq k_{1}\left(\Gamma^{\prime}\right)$.
Repeatedly attach all inner vertices to obtain a stower with $E_{l}$ leaves and $E-E_{l}$ petals.
Use bound on stowers: $k_{1}[\Gamma] \leq \pi\left(E-\frac{E_{l}}{2}\right) \quad$ [to appear in a future slide]

## Spectral gap as a simple eigenvalue - Critical points

Try to find supremizers by seeking for local critical points in $\mathscr{L}_{\mathcal{G}}$.
Derivatives with respect to edge lengths may be calculated for simple eigenvalues.
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Theorem 5 (Band, Lévy).
Let $\mathcal{G}$ be a discrete graph and $\underline{I} \in \mathscr{L}_{\mathcal{G}}$
Assume that $\Gamma\left(\mathcal{G} ; \Omega\right.$ is a sunremizer of $\mathcal{G}$ with simple spectral gap $k_{1}[\Gamma(\mathcal{G} ; I)]$.
Then $\Gamma(\mathcal{G} ; \underline{1})$ is not a unique supremizer:
there exists $\underline{I}^{*} \in \mathscr{L}_{\mathcal{G}}$ s.t. $\Gamma\left(\mathcal{G} ; \underline{I}^{*}\right)$ is an equilateral mandarin and

$$
k_{1}\left[\Gamma\left(g_{i}, I\right)\right]=k_{1}\left[\Gamma\left(g_{i} I^{*}\right)\right]
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Proof ingredients.

- A supremizer is a critical point of some $\mathscr{L}_{\hat{\mathcal{C}}}(\hat{\mathcal{G}}$ maybe different than $\mathcal{G})$
- $\forall e \frac{\partial}{\partial l_{e}}\left(k^{2}\right)=-\left.\left(f^{\prime 2}+k^{2} f^{2}\right)\right|_{e}$ where $f$ eigenfunction which corresponds to $k$.
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- This implies restrictions on eigenfunction derivatives.
- Courant nodal domain theorem - $f$ has exactly two nodal domains.


## Gluing graphs - Vertex connectivity one

Let $\mathcal{G}_{1}, \mathcal{G}_{2}$ be discrete graphs, and $v_{i}(i=1,2)$ be a vertex of $\mathcal{G}_{i}$. Let $\mathcal{G}$ be the graph obtained by identifying (gluing) $v_{1}$ and $v_{2}$. If we know the supremizers $\Gamma_{1}, \Gamma_{2}$ of $\mathcal{G}_{1}, \mathcal{G}_{2}$, can we tell the supremizer of $\mathcal{G}$ ?


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Yes (under some conditions on $k_{1}\left(\Gamma_{1}\right), k_{1}\left(\Gamma_{2}\right)$ )
For brevity, skip here the theorem and move on to its corollaries.
Corollary 6.
Let $\mathcal{G}_{1}, \mathcal{G}_{2}$ be discrete graphs.
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If the (unique) supremizer of $\mathcal{G}_{i}$ is the "equilateral" stower
with $E_{\rho}^{(i)}$ petals and $E_{l}^{(i)}$ leaves, such that $E_{\rho}^{(i)}+E_{l}^{(i)} \geq 2$, then the (unique) supremizer of $\mathcal{G}$ is an "equilateral" stower with $E_{p}^{(1)}+E_{p}^{(2)}$ petals and $E_{l}^{(1)}+E_{l}^{(2)}$ leaves.

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## Gluing graphs - Corollaries

## Corollary 7.

Let $\mathcal{G}$ be a stower with $E_{p}+E_{l} \geq 2$ and $\left(E_{p}, E_{l}\right) \neq(1,1)$. Then a maximizer is the "equilateral" stower graph with spectral gap $\pi\left(E_{p}+\frac{E_{l}}{2}\right)$. This maximizer is unique for $\left(E_{p}, E_{l}\right) \notin\{(2,0),(1,2)\}$.

Prove the statement for "small" stowers. Then glue them to construct any stower

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## Proposition 4:

Let $\mathcal{G}$ be a graph with $E$ edges, out of which $E_{I}$ are leaves.
If $\left(E, E_{l}\right) \notin\{(1,1),(1,0),(2,1)\}$ then $\forall \underline{I} \in \mathscr{L}_{\mathcal{G}}, \quad k_{1}[\Gamma(\mathcal{G} ; \underline{I})] \leq \pi\left(E-\frac{E_{I}}{2}\right)$.
Assuming $\left(E, E_{l}\right) \notin\{(2,0),(3,2)\}$ equality above implies $\Gamma(\mathcal{G} ; \underline{l})$ is
either an equilateral mandarin $\left(E_{I}=0\right)$ or an equilateral stower $\left(E_{I} \geq 0\right)$.
We use Corollary 7 in its proof.

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- Optimization problem fully solved for infimizers $\backslash$ minimizers.
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Supremizer candidates are stowers and mandarins (are there any others?)
$\Rightarrow$ lower bounds on supremal spectral gap

Getting to a stower gives $\pi\left(\beta+\frac{E_{l}}{2}\right)$,
where $\beta:=E-V+1$ is the graph's first Betti number.
Getting to a mandarin:
Partition vertices $V=V_{1} \cup V_{2}$.
$E\left(V_{1}, V_{2}\right):=\#$ of edges connecting $V_{1}$ to $V_{2}$
Maximal spectral gap among all mandarins is
$\pi \cdot \max _{V_{1}, V_{2}} E\left(V_{1}, V_{2}\right) \cdot$ (Cheeger-like constant)
Compare $\pi\left(\beta+\frac{E_{1}}{2}\right)$ (stower) with $\pi \cdot \max _{V_{1}, V_{2}} E\left(V_{1}, V_{2}\right)$ (mandarin).
$E\left(V_{1}, V_{2}\right)=\beta+1-\left(\beta_{1}+\beta_{2}\right)$, where $\beta_{i}$ is the Betti number of $V_{i}$ graph.
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$\longrightarrow$
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Leads to conjectures....

## Conjectures

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## Quantum Graphs which Optimize the Spectral Gap



Ram Band<br>Technion - Israel Institute of Technology

Joint work with Guillaume Lévy, Université Pierre et Marie Curie, Paris (arXiv:1608.00520)

QMath 13, GeorgiaTech, Atlanta - October 2016

