Infinite Quantum Graphs

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FWF Der Wissenschaftsfonds.

Combinatorial and Metric Graphs

Definition

A (combinatorial) graph is the set of vertices $\mathcal{V}$ and edges $\mathcal{E}$, $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$.

For $u, v \in \mathcal{V}$ we shall write $u \sim v$ if there is $e_{u,v} \in \mathcal{E}$ connecting u and v. The function $\deg\colon \mathcal{V} \to \mathbb{Z}_{\geq 1} \cup \{\infty\}$ defined by

$$\deg\colon v \mapsto \#\{u \in \mathcal{V} |\, u \sim v\} = \#\mathcal{E}_v$$

is called the (combinatorial) degree, where $\mathcal{E}_v := \{e_{u,v} \in \mathcal{E} |\, u \sim v\}$.

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If every edge $e \in \mathcal{E}$ is assigned with a length $|e| \in (0, \infty)$, then $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$ is called a metric graph

Quantum Graphs

Given a metric graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$, we can identify each edge $e \in \mathcal{E}$ with an interval $(0, |e|)$ and hence introduce the Hilbert space

$$L^2(\mathcal{G}) := \bigoplus_{e\in\mathcal{E}} L^2(e) = \Big\{ f = \{f_e\}_{e\in\mathcal{E}} \colon f_e \in L^2(e),\ \sum_{e\in\mathcal{E}} \|f_e\|^2_{L^2(e)} < \infty \Big\}$$

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Given a metric graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$, we can identify each edge $e \in \mathcal{E}$ with an interval $(0, |e|)$ and hence introduce the *weighted* Hilbert space

$$L^2(\mathcal{G}; \mu) := \bigoplus_{e\in\mathcal{E}} L^2(e; \mu_e)$$

Next equip $\mathcal{G}$ with a Schrödinger-type operator $\mathbf{H}_{\max} := \bigoplus_{e\in\mathcal{E}} \mathrm{H}_e$, where:

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$$f_e(v) := \lim_{x_e\to v} f(x_e), \qquad f_e'(v) := \lim_{x_e\to v} \frac{f(x_e) - f_e(v)}{|x_e - v|}.$$

are well defined for all $f \in \mathrm{dom}(\mathbf{H}_{\mathrm{max}})$.

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(standard) Kirchhoff conditions: For all $v \in \mathcal{V}$

$$\begin{cases} f \text{ is continuous at } v, \\ \sum_{e\in\mathcal{E}_v} f_e'(v) = 0. \end{cases}$$

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Definition

A quantum graph is a metric graph equipped with the operator $\mathbf{H}$ acting as the negative second order derivative along edges and accompanied by Kirchhoff vertex conditions

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Define the normalized/physical Laplacian on $\mathcal{G}_d$ by

$$(\tau_{\rm norm} f)(v) := \frac{1}{\deg(v)} \sum_{u\sim v} f(v) - f(u), \quad v \in \mathcal{V}.$$

$\tau_{\rm norm}$ generates a bounded self-adjoint operator $h_{\rm norm}$ in $\ell^2(\mathcal{V}; \deg)$.

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Y. Colin de Verdiére, *Spectres de Graphes*, SMF, Paris, 1998.

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Theorem (von Below'87,..., Cattaneo, Exner,..., Pankrashkin'2012)

$$\sigma_j(\mathbf{H}_{\mathrm{equil}}) \setminus \sigma_D = \{\lambda \notin \sigma_D |\ 1 - \cos(\sqrt{\lambda}) \in \sigma_j(h_{\mathrm{norm}})\}, \quad j \in \{\mathrm{p}, \mathrm{ess}, \mathrm{ac}, \mathrm{sc}\}$$

with $\sigma_D = \{(\pi n)^2\}_{n \in \mathbb{N}}$.

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Consider the (minimal) discrete Laplacian $h_{\mathcal{G}}$ defined on $\ell^2(\mathcal{V}; m)$ by

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$\boxed{\tau_{\mathcal{G}} \text{ is the normalized Laplacian } \textbf{iff } |e| = 1 \text{ for all } e \in \mathcal{E} \text{ and } \alpha \equiv 0}$.

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$h_{\mathcal{G}}$ is bounded $\Leftrightarrow$ the weighted degree Deg is bounded on $\mathcal{V}$,

$$\mathrm{Deg}\colon v \mapsto \frac{1}{m(v)} \sum_{u \sim v} \frac{1}{|e_{u,v}|} = \frac{\sum_{e \in \mathcal{E}_v} 1/|e|}{\sum_{e \in \mathcal{E}_v} |e|}$$

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Note that Deg is bounded on $\mathcal{V}$ if $\ell_*(\mathcal{E}) := \inf_{e\in\mathcal{E}} |e| > 0.$

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Theorem 1 (Exner, AK, Malamud, Neidhardt'2018)

Let $\mathcal{G}$ be a metric graph with $\ell^*(\mathcal{G}) := \sup_{e\in\mathcal{E}} |e| < \infty$. Then:

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(v)

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for some $D > 2$ if and only if

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P. Exner, A. Kostenko, M. Malamud, & H. Neidhardt, *Spectral theory of infinite quantum graphs*, Ann. Henri Poincaré **19**, no. 11, (2018).

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A. Kostenko and N. Nicolussi, *Spectral estimates for infinite quantum graphs*, Calc. Var. Partial Differential Equations **58**, no. 1, (2019).

Quantum Graphs: Self-adjointness

For $p\colon \mathcal{E} \to (0,\infty)$, define a path metric ϱ_p on $\mathcal{V}$ w.r.t. $\mathcal{G}$ by

$$\varrho_p(u,v) := \inf_{\mathcal{P}=\{v_0,\dots,v_n\}\colon\ u=v_0,\ v=v_n} \sum_k p(e_{v_{k-1},v_k}).$$

The infimum is taken over all paths connecting u and v.

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- Natural path metric ϱ_0 with $p_0\colon e \mapsto |e|$.
- Star metric ϱ_m with $p_m\colon e_{u,v} \mapsto m(u) + m(v)$ with $m(v) = \sum_{e\in\mathcal{E}_v} |e|$

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Hopf–Rinow-type Theorem

$(\mathcal{V}, \varrho_p)$ is complete as a metric space $\Longleftrightarrow$
$(\mathcal{V}, \varrho_p)$ is geodesically complete $\Longleftrightarrow$
The distance balls in $(\mathcal{V}, \varrho_p)$ are finite (*"finite ball condition"*).

X. Huang, M. Keller, J. Masamune, R. Wojciechowski, *A note on self-adjoint extensions of the Laplacian on weighted graphs*, J. Funct. Anal. **265** (2013).

Quantum Graphs: Self-adjointness

For $p\colon \mathcal{E} \to (0,\infty)$, define a path metric ϱ_p on $\mathcal{V}$ w.r.t. $\mathcal{G}$ by

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M. Keller and D. Lenz, *Dirichlet forms and stochastic completeness of graphs and subgraphs*, J. reine angew. Math. **666** (2012).

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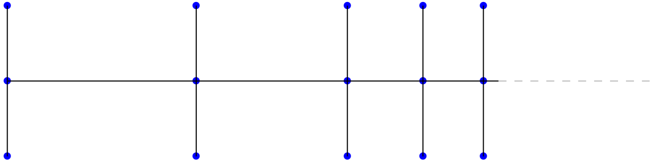
The standard assumption for infinite QG is $\inf_{e\in\mathcal{E}} |e| > 0$!

Quantum Graphs: Self-adjointness

Example 1.



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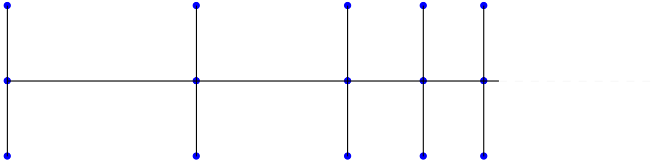

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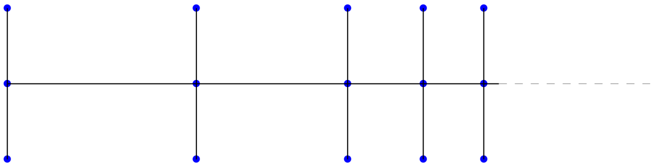

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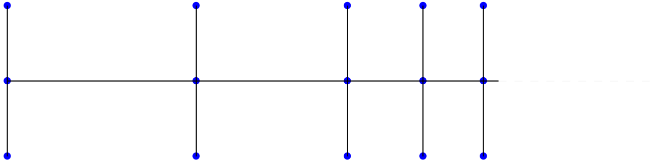

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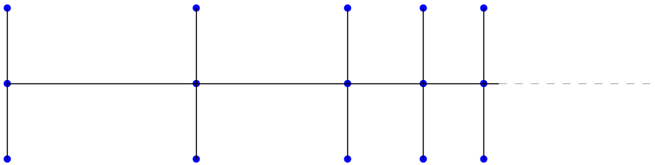

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The converse to Theorem 2 is not true!

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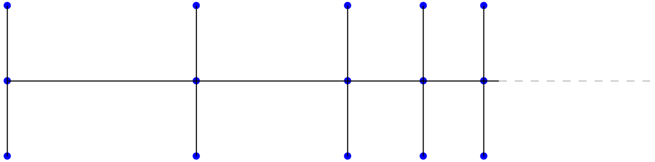

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For radially symmetric trees and antitrees, **H** is self-adjoint $\Leftrightarrow$ $m(\mathcal{V}) = \infty$.

Examples: Radially symmetric antitrees

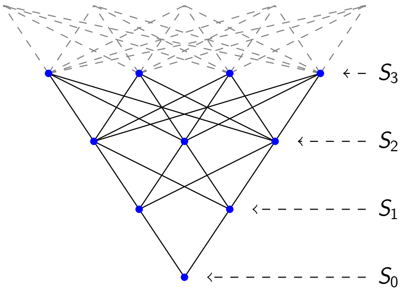
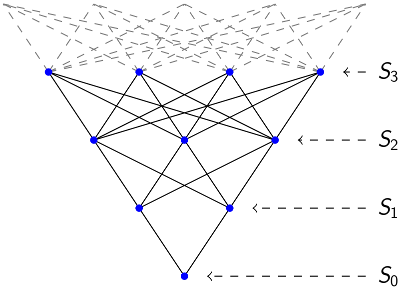


Figure: Example of an antitree $\mathcal{A}$ with $s_n = n + 1$.

S_n is the n-th combinatorial sphere, and $s_n := \#S_n$.
$\mathcal{A}$ is radially symmetric if edges connecting S_n with S_{n+1} have the same length, say ℓ_n, for all $n \geq 0$.



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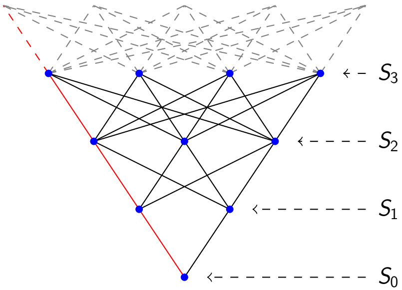

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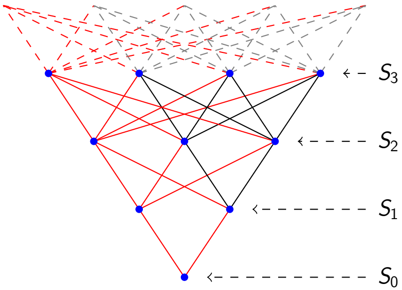

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$(\mathcal{A}, \varrho_0)$ is complete $\iff \sum_{n\geq 0} \ell_n = \infty$.
$(\mathcal{V}, \varrho_m)$ is complete $\iff \sum_{n\geq 0} (s_n + s_{n+1}) \ell_n = \infty$

Quantum Graphs: Self-adjointness

Summary

(i) $\mathbf{H}$ is self-adjoint if $(\mathcal{V}, \varrho_m)$ is complete.

(ii) $\mathbf{H}$ is non-self-adjoint if $\mathrm{vol}(\mathcal{G}) = \sum_{e \in \mathcal{E}} |e| < \infty$.

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(i) Characterize metric graphs such that completeness of $(\mathcal{V}, \varrho_m)$ is also necessary for self-adjointness.

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$\mathrm{vol}(\mathcal{G}) = \sum_{e\in\mathcal{E}} |e| < \infty$, then **H** is non-self-adjoint

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Graph Ends

- A *ray* R in $\mathcal{G}_d$ is a path without intersections.
- Two rays are *equivalent* if there is a third ray containing infinitely many vertices of both rays.
- An equivalence class of rays is a *graph end*; $\Omega(\mathcal{G}_d)$ is the set of graph ends.

Theorem (e.g., Diestel–Kühn '2003)

Topological ends of $\mathcal{G}$ = graph ends of $\mathcal{G}_d$.

Graph Ends: Examples

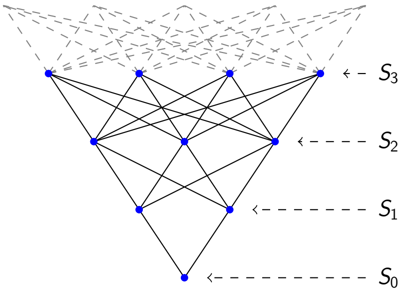

Figure: An antitree $\mathcal{A}$ with $s_n = n + 1$.

Every antitree has exactly 1 end.

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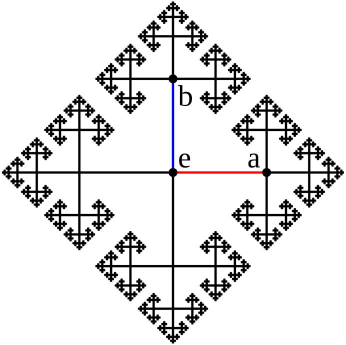

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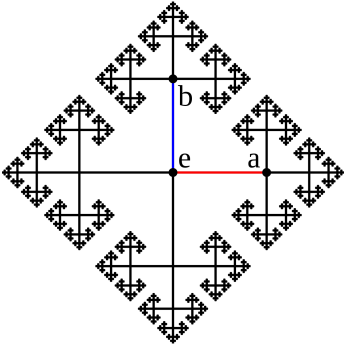

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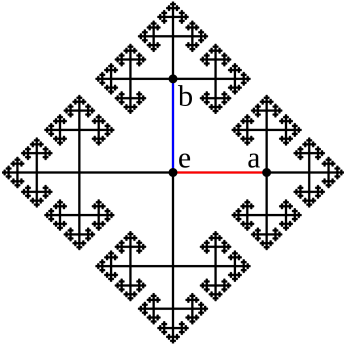

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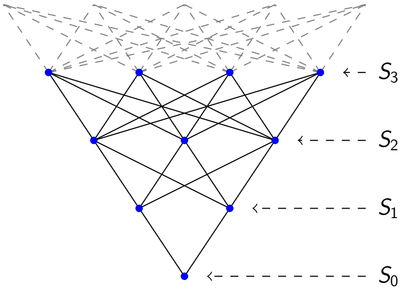

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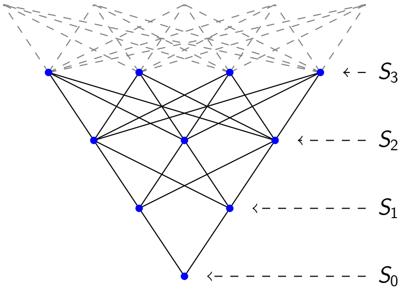

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However, there are antitrees with $n_{\pm}(\mathcal{A}) = \infty$!

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Theorem (AK–Mugnolo–Nicolussi, *in preparation*)

If $\mathrm{vol}(\mathcal{G}) < \infty$, then $n_\pm(\mathbf{H}) \ge \#\Omega(\mathcal{G}_d)$. Moreover, $n_\pm(\mathbf{H}) = \#\Omega(\mathcal{G}_d)$ if and only if either $\#\Omega(\mathcal{G}_d) = \infty$ or $\ker(\mathbf{H}^*) \subset H^1(\mathcal{G})$.

Here $H^1(\mathcal{G})$ is the usual Sobolev space on $\mathcal{G}$.

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- $H^1(\mathcal{G})$ is a 'nice' space (e.g., graph ends can be identified with its Royden's boundary, which gives a hope for reasonable traces of functions in $\mathrm{dom}(\mathbf{H}^*)$).

In the discrete setting, see

A. Georgakopoulos, S. Haeseler, M. Keller, D. Lenz and R. Wojciechowski, *Graphs of finite measure*, J. Math. Pures Appl. **103** (2015).

Weighted Quantum Graphs

Given a metric graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$.
Suppose we are given two more edge weights

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Introduce the *weighted* Hilbert space $L^2(\mathcal{G};\mu) := \bigoplus_{e\in\mathcal{E}} L^2(e;\mu_e)$
and equip $\mathcal{G}$ with a Schrödinger-type operator $\mathbf{H}_{\max} := \bigoplus_{e\in\mathcal{E}} \mathrm{H}^e_{\mu,\nu}$, where:

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The operator $\mathbf{H}_{\mu,\nu}$ with Kirchhoff conditions: For all $v \in \mathcal{V}$

$$\begin{cases} f \text{ is continuous at } v, \\ \sum_{e\in\mathcal{E}_v} \nu_e f_e'(v) = 0. \end{cases}$$

Weighted Quantum Graphs

The analog of Theorem 1 for $\mathbf{H}_{\mu,\nu}$ holds true, however, with the (minimal) discrete Laplacian defined on $\ell^2(\mathcal{V}; m_\mu)$ by

$$(\tau_{\mathcal{G}} f)(v) := \frac{1}{m_\mu(v)} \sum_{u\sim v} b_\nu(e_{u,v})(f(v) - f(u)),$$

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Remark (self-adjointness)

If $\mathcal{G}$ is a path graph, then $\mathbf{H}_{\mu,\nu}$ is self-adjoint if and only if

$$\sum_n \mu_n|e_n|\Big(\sum_{k\le n} \frac{|e_k|}{\nu_k}\Big)^2 = \infty.$$

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If $\mathcal{G}$ is a path graph, then $\mathbf{H}_{\mu,\nu}$ is self-adjoint if and only if

$$\sum_n \mu_n|e_n|\Big(\sum_{k\le n} \frac{|e_k|}{\nu_k}\Big)^2 = \infty.$$

Hence $\sum m_\mu(v_n) = 2\sum \mu_n|e_n| = \infty$ is only sufficient!

Weighted Quantum Graphs

The analog of Theorem 1 for $\mathbf{H}_{\mu,\nu}$ holds true, however, with the (minimal) discrete Laplacian defined on $\ell^2(\mathcal{V}; m_\mu)$ by

$$(\tau_{\mathcal{G}} f)(v) := \frac{1}{m_\mu(v)} \sum_{u \sim v} b_\nu(e_{u,v})(f(v) - f(u)),$$

where

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Weighted discrete Laplacian

For $m\colon \mathcal{V} \to \mathbb{R}_{>0}$ and $b\colon \mathcal{E} \to \mathbb{R}_{>0}$, consider in $\ell^2(\mathcal{V}; m)$

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QUESTION: For a given τ (i.e., a pair of functions m and b), does there exist a "weighted" $\mathcal{G}$ (i.e., weights $|\cdot|$, μ and ν) such that $\tau = \tau_{\mathcal{G}}$?

Weighted Quantum Graphs: Examples

Normalized/Physical Laplacian

Take $\mu_e = \nu_e = |e|$ for all $e \in \mathcal{E}$, then

$$m_\mu(v) = \deg(v), \qquad b_\nu(e) = 1.$$

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Electric Networks/Random Walks on Graphs

Take $\nu_e = |e|b(e)$ and $\mu_e = \frac{b(e)}{|e|}$ for all $e \in \mathcal{E}$, then

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Path Graphs and Jacobi Matrices

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Path Graphs and Jacobi Matrices

Every Jacobi matrix can be realized as a boundary operator for a weigthed quantum path graph (with δ-interactions at the vertices)

Weighted Quantum Graphs

Combinatorial Laplacian: $m \equiv 1$, $b \equiv 1$

$$(\tau_{\mathrm{comb}} f)(v) := \sum_{u \sim v} f(v) - f(u) = \deg(v) f(v) - \underbrace{\sum_{u \sim v} f(u)}_{adjacency\ \ matrix} .$$

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If $\mathcal{G}_d$ has loose ends, then one can't construct a metric with $\mathbf{H}_{\mu,\nu}$!
For an antitree $\mathcal{A}$, only if $\sum_{k=0}^{n}(-1)^k s_{n-k} > 0$ for all $n \geq 0$.

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Theorem (G. Zaimi '2011: mathoverflow.net/questions/59117)

Let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be simple, connected, locally finite. Then there are lengths $|\cdot|\colon \mathcal{E} \to \mathbb{R}_{>0}$ and weights $\mu\colon \mathcal{E} \to \mathbb{R}_{>0}$ such that

$$\sum_{e\in\mathcal{E}_v} \mu(e)|e| = 1 \quad \text{for all} \quad v \in \mathcal{V},$$

if and only if for each $e \in \mathcal{E}$ there is a disjoint cycle cover containing e in one of its cycles.

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The way to fix this problem is to allow loops!

M. Folz, *Volume growth and stochastic completeness of graphs*, Trans. Amer. Math. Soc. **366** (2014).

X. Huang, *A note on the volume growth criterion for stochastic completeness of weighted graphs*, Potential Anal. **40** (2014).

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If $\mathcal{G}_d$ has loose ends, then one can't construct a metric with $\mathbf{H}_{\mu,\nu}$!
For an antitree $\mathcal{A}$, only if $\sum_{k=0}^{n}(-1)^k s_{n-k} > 0$ for all $n \geq 0$.

The way to fix this problem is to allow loops!
Then every weighted discrete Laplacian can be realized as a boundary operator for a quantum graph operator (in the sense of Theorem 1), however, the metric graph might be with loops.

A. Kostenko, M. Malamud, and N. Nicolussi, *Weighted quantum graphs*, in preparation.

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Thank you for your attention!