Spectral Estimates for Infinite Quantum Graphs

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(joint work with N. Nicolussi)

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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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Definition

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

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

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

$$\mathrm{H}_e = -\frac{\mathrm{d}^2}{\mathrm{d}x_e^2}, \qquad \mathrm{dom}(\mathrm{H}_e) = H^2(e).$$

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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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To give $\mathbf{H}$ the meaning of a quantum mechanical energy operator, it must be self-adjoint, that is, we need to add boundary conditions at the vertices.

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

Infinite Graphs ($\#\mathcal{V}$, $\#\mathcal{E} = \infty$)

Assumptions

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Theorem (M. Solomyak'2003)

If $\ell^*(\mathcal{E}) = \infty$, then

$$\hat{\sigma}(\mathbf{H}) = \mathbb{R}_{\geq 0}.$$

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PROBLEM #1:

The (minimal) operator **H** is symmetric, however, in contrast to the case of finite graphs, it is not necessarily self-adjoint!

Infinite 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

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

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Examples

- Natural path metric ϱ_0 with $p_0\colon e \mapsto |e|$.
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If $(\mathcal{V}, \varrho_m)$ is complete as a metric space, then $\mathbf{H}$ is self-adjoint.

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Corollary ([EKMN])

If $(\mathcal{G},\varrho_0)$ is complete as a metric space, then $\mathbf{H}_{\mathcal{G}}$ is self-adjoint.

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M. Keller and D. Lenz// J. reine Angew. Math. **666**, 189–223 (2012).

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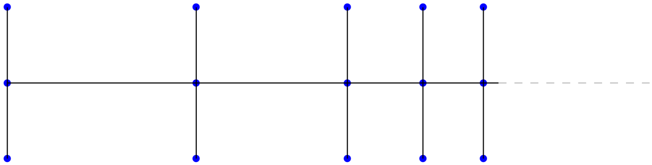

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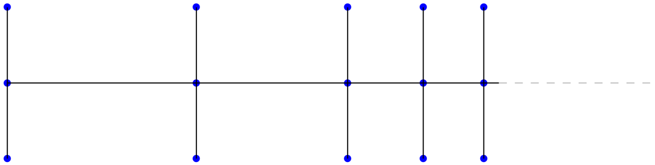

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Example 1, $(\mathcal{V}, \varrho_m)$ is complete $\Leftrightarrow L := \sum_{e\in\mathcal{E}} |e| = \frac{1}{2}m(\mathcal{V}) = \infty$.

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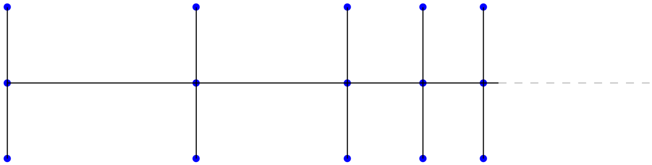

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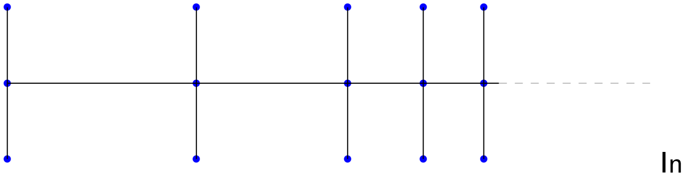

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Hence, in Example 1, $\boxed{\mathbf{H} \text{ is self-adjoint} \Leftrightarrow (\mathcal{V}, \varrho_m) \text{ is complete!}}$

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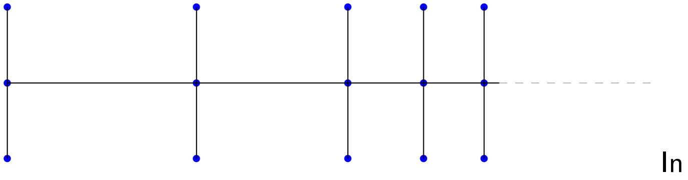

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Open Problem:

Does the converse to Theorem 1 hold true in general?

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

$$(\tau f)(v) := \frac{1}{m(v)} \sum_{u \sim v} \frac{f(v) - f(u)}{|e_{u,v}|}, \quad v \in \mathcal{V}.$$

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τ is the combinatorial Laplacian iff $\mathcal{G}$ is equilateral, i.e., $|e| \equiv 1$.

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

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Theorem (E. B. Davies'1992)

h is bounded iff the weighted degree Deg is bounded on $\mathcal{V}$,

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

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

Connections between $\mathbf{H}$ and h

The kernel $\mathcal{L} = \ker(\mathbf{H}_{\max})$ consists of piecewise linear functions on $\mathcal{G}$.
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Now restrict ourselves to the subspace $\mathcal{L}_{cont} = \mathcal{L} \cap C_c(\mathcal{G})$. Clearly,

$$\sum_{e\in\mathcal{E}} |e|(|f(e_i)|^2 + |f(e_o)|^2) = \sum_{v\in\mathcal{V}} |f(v)|^2 \underbrace{\sum_{e\in\mathcal{E}_v} |e|}_{=m(v)} = \|f\|^2_{\ell^2(\mathcal{V};m)}$$

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defines an equivalent norm on $\mathcal{L}_{cont}$. Moreover, for $f \in \mathcal{L}_{cont}$

$$(\mathbf{H}f, f)_{L^2(\mathcal{G})} = \sum_{e\in\mathcal{E}} \int_e |f'(x_e)|^2 dx_e = \sum_{e\in\mathcal{E}} \frac{|f(e_o) - f(e_i)|^2}{|e|}$$

$$= \frac{1}{2} \sum_{u,v\in\mathcal{V}} \frac{|f(v) - f(u)|^2}{|e_{u,v}|} = \big(\mathrm{h}f, f\big)_{\ell^2(\mathcal{V};m)}.$$

Connections between $\mathbf{H}$ and h

For $f \in \mathcal{L}_{cont} = \ker(\mathbf{H}_{\max}) \cap C_c(\mathcal{G})$,

$$(\mathbf{H}f, f)_{L^2(\mathcal{G})} = (\mathrm{h}f, f)_{\ell^2(\mathcal{V};m)}$$

and

$$\frac{1}{6}\|f\|^2_{\ell^2(\mathcal{V};m)} \le \|f\|^2_{L^2(\mathcal{G})} \le \frac{1}{2}\|f\|^2_{\ell^2(\mathcal{V};m)}$$

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Rayleigh's quotient

$$\lambda_0(\mathbf{H}) := \inf \sigma(\mathbf{H}) = \inf_{\substack{f \in H^1_c(\mathcal{G}) \\ f \neq 0}} \frac{(\mathbf{H}f, f)_{L^2(\mathcal{G})}}{\|f\|^2_{L^2(\mathcal{G})}} \le \inf_{\substack{f \in \mathcal{L}_{cont} \\ f \neq 0}} \frac{(\mathbf{H}f, f)_{L^2(\mathcal{G})}}{\|f\|^2_{L^2(\mathcal{G})}} \le 6\lambda_0(\mathrm{h}).$$

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Theorem (von Below'1987,..., Cattaneo'1997,..., Pankrashkin'2012)

Let $\mathcal{G}$ be equilateral ($|e| = 1$ for all $e \in \mathcal{E}$) and $\sigma_D := \{(\pi n)^2\}_{n \in \mathbb{N}}$. Then

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

Connections between $\mathbf{H}$ and h

For $f \in \mathcal{L}_{cont} = \ker(\mathbf{H}_{\max}) \cap C_c(\mathcal{G})$,

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Corollary

Let $\mathcal{G}$ be equilateral. Then $\lambda_0(\mathbf{H}) = 1 - \cos(\sqrt{\lambda_0(\mathrm{h})})$. In particular,

$$2\lambda_0(\mathrm{h}) \le \lambda_0(\mathbf{H}) \le \frac{\pi^2}{4}\lambda_0(\mathrm{h})$$

Connections between $\mathbf{H}$ and h

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Theorem 2 (Exner–AK–Malamud–Neidhardt)

$$\lambda_0(\mathbf{H}) > 0 \quad \Leftrightarrow \quad \lambda_0(\mathrm{h}) > 0$$

However, there is no nice formula like in the equilateral case!

Estimates for $\lambda_0(\mathbf{H})$

A huge literature in the case of finite graphs.

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One can use volume growth estimates, aka Brooks-type bounds, since $\mathfrak{t}_{\mathbf{H}}[\cdot] = (\mathbf{H}\cdot,\cdot)_{L^2}$ is a regular local Dirichlet form and ϱ_0 is intrinsic:

K.-T. Sturm, *Analysis on local Dirichlet spaces I. Recurrence, conservativeness and L^p-Liuoville properties*, J. reine Angew. Math. **456**, 173–196 (1994).

Cheeger-type estimates for $\lambda_0(\mathbf{H})$

Let $\mathcal{K}_{\mathcal{G}}$ be the set of all finite, connected subgraphs of $\mathcal{G}$.
For $\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}$, *the boundary of $\widetilde{\mathcal{G}}$* (w.r.t.$\mathcal{G}$) is

$$\partial_{\mathcal{G}}\widetilde{\mathcal{G}} := \big\{ v \in \tilde{\mathcal{V}} \,|\, \deg_{\widetilde{\mathcal{G}}}(v) < \deg_{\mathcal{G}}(v) \big\}.$$

For a given finite subgraph $\widetilde{\mathcal{G}} \subset \mathcal{G}$ we then set

$$\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}) := \sum_{v \in \partial\widetilde{\mathcal{G}}} \deg_{\widetilde{\mathcal{G}}}(v).$$

The Cheeger (or isoperimetric) constant of a metric graph $\mathcal{G}$ is defined by

$$\alpha(\mathcal{G}) := \inf_{\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}} \frac{\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}})}{\mathrm{mes}(\widetilde{\mathcal{G}})},$$

where $\mathrm{mes}(\widetilde{\mathcal{G}})$ denotes the Lebesgue measure of $\widetilde{\mathcal{G}}$, $\mathrm{mes}(\widetilde{\mathcal{G}}) := \sum_{e \in \widetilde{\mathcal{E}}} |e|$.

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Theorem 3 (AK–Nicolussi)

$$\lambda_0(\mathbf{H}) \geq \tfrac{1}{4}\alpha(\mathcal{G})^2$$

Cheeger-type estimates for $\lambda_0(\mathbf{H})$

The Cheeger inequality for finite graphs was proved in

S. Nicaise, *Spectre des réseaux topologiques finis*, Bull. Sci. Math., **II.** Sér., **111**, 401–413 (1987).

However, the isoperimetric constant is defined (for finite graphs) by

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In fact, for infinite graphs (having infinite total length)

$$\boxed{\widetilde{\alpha}(\mathcal{G}) = \alpha(\mathcal{G})}$$

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The discrete isoperimetric constant for h was introduced in

F. Bauer, M. Keller, and R. K. Wojciechowski, *Cheeger inequalities for unbounded graph Laplacians*, J. Eur. Math. Soc. **17**, 259–271 (2015).

$$\alpha_d(\mathcal{V}) := \inf_{\substack{X \subseteq \mathcal{V} \\ X \text{ is finite}}} \frac{\#(\{e \in \mathcal{E} \,|\, e \text{ connects } X \text{ and } \mathcal{V} \setminus X\})}{\sum_{v \in X} m(v)}$$

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Lemma (AK–Nicolussi)

$$\frac{1}{\alpha_d(\mathcal{V})} \leq \frac{2}{\alpha(\mathcal{G})} \leq \frac{1}{\alpha_d(\mathcal{V})} + \ell^*(\mathcal{G})$$

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In particular, this implies $\lambda_0(\mathbf{H}) > 0$ if $\alpha_d(\mathcal{V}) > 0$.

Cheeger-type estimates for $\lambda_0(\mathbf{H})$

The combinatorial isoperimetric constant of a graph $\mathcal{G}_d$ was introduced in

J. Dodziuk and W. S. Kendall, *Combinatorial Laplacians and isoperimetric inequality*, in: K. D. Elworthy (ed.), "From local times to global geometry, control and physics", pp. 68–74, 1986.

$$\alpha_{\mathrm{comb}}(\mathcal{G}) := \inf_{\substack{X \subseteq \mathcal{G} \\ X \text{ is finite}}} \frac{\#(\{e \in \mathcal{E} |\ e \text{ connects } X \text{ and } \mathcal{V} \backslash X\})}{\sum_{v \in X} \deg(v)}.$$

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It is easy to see that

$$\frac{\alpha_{\mathrm{comb}}(\mathcal{V})}{\ell^*(\mathcal{G})} \le \alpha_d(\mathcal{V}) \le \frac{\alpha_{\mathrm{comb}}(\mathcal{V})}{\ell_*(\mathcal{G})}.$$

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and hence

$$\frac{2\,\alpha_{\rm comb}(\mathcal{V})}{\ell^*(\mathcal{G})(1+\alpha_{\rm comb}(\mathcal{V}))} \le \alpha(\mathcal{G}) \le \frac{2\,\alpha_{\rm comb}(\mathcal{V})}{\ell_*(\mathcal{G})}.$$

In particular, this implies $\lambda_0(\mathbf{H}) > 0$ if $\alpha_{\rm comb}(\mathcal{V}) > 0$ and $\ell^*(\mathcal{G}) < \infty$.

Buser-type estimates for $\lambda_0(\mathbf{H})$

Bounds from above via isoperimetric constants:

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Theorem 4 (AK–Nicolussi)

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This estimate becomes trivial if $\ell_*(\mathcal{E}) = \inf |e| = 0$.

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Corollary (AK–Nicolussi)

If $\ell^*(\mathcal{E}) = \sup |e| < \infty$ and $\ell_*(\mathcal{E}) = \inf |e| > 0$, then

$$\boxed{\lambda_0(\mathbf{H}) > 0 \quad \Leftrightarrow \quad \alpha(\mathcal{G}) > 0 \quad \Leftrightarrow \quad \alpha_{\mathrm{comb}}(\mathcal{G}) > 0}$$

Examples: Trees

A connected graph without cycles is called *a tree*.

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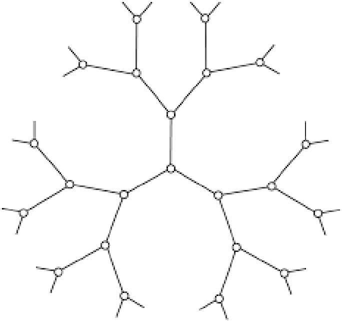

Bethe lattice (Cayley tree or regular tree $\mathbb{T}_3$)

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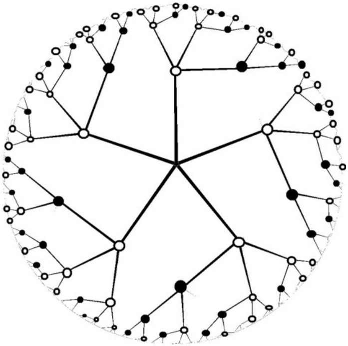

Spanning tree for the hyperbolic (4,5)-tessellation

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$$\ell^*_{\mathrm{ess}}(\mathcal{G}) := \limsup_{e\in\mathcal{E}} |e|,$$

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Theorem 5 (AK–Nicolussi)

Assume $\mathcal{G}$ is a rooted tree without loose ends. Then

$$\lambda_0(\mathbf{H}) \ge \frac{\mathrm{K}(\mathcal{G})^2}{4\,\ell^*(\mathcal{G})^2}, \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \ge \frac{\mathrm{K}_{\mathrm{ess}}(\mathcal{G})^2}{4\,\ell^*_{\mathrm{ess}}(\mathcal{G})^2}.$$

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In particular, $\lambda_0(\mathbf{H}) > 0$ if and only if $\ell^*(\mathcal{G}) < \infty$ and
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For radial trees this was proved by M. Solomyak in 2004.

Examples: Antitrees

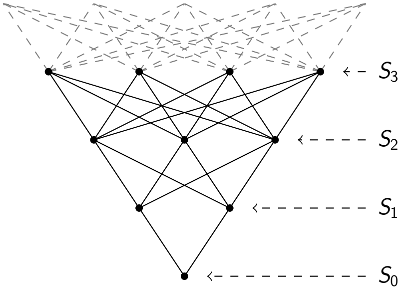

Figure: Example of an antitree with $s_n = n + 1$.

S_n is the n-th combinatorial sphere, and
$s_n := \# S_n$ is the number of vertices in S_n.

Examples: Antitrees

Set $\ell_n := \sup_{v\in S_n,\ u\in S_{n+1}} |e_{u,v}|$ for all $n \in \mathbb{Z}_{\geq 0}$, and

$$\mathrm{K}_0 := 1, \qquad \mathrm{K}_{n+1} := 1 - \frac{s_n}{s_{n+2}}, \quad n \in \mathbb{Z}_{\geq 0}.$$

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Theorem 6 (AK–Nicolussi)

Let $\mathcal{G} = \mathcal{A}$ be an antitree. Then

$$\lambda_0(\mathbf{H}) \geq \frac{1}{4}\mathrm{K}(\mathcal{A})^2, \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \geq \frac{1}{4}\mathrm{K}_{\mathrm{ess}}(\mathcal{A})^2.$$

where

$$\mathrm{K}(\mathcal{A}) := \inf_{n\geq 0} \tfrac{\mathrm{K}_n}{\ell_n} \quad \text{and} \quad \mathrm{K}^{\mathrm{ess}}(\mathcal{A}) := \liminf_{n\to\infty} \tfrac{\mathrm{K}_n}{\ell_n}.$$

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In particular, if $\inf_n \mathrm{K}_n > 0$, then:

(i) $\lambda_0(\mathbf{H}) > 0$ if and only if $\ell^*(\mathcal{G}) < \infty$,

(ii) the spectrum of $\mathbf{H}$ is purely discrete if and only if $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$.

Examples: An antitree with $\alpha_{\mathrm{comb}} = 0$ and $\ell_* = 0$

Consider a particular example: fix $q \in \mathbb{Z}_{\geq 1}$ and $s \in \mathbb{R}_{\geq 0}$ and set

$$s_n = (n+1)^q, \qquad |e_{u,v}| = (n+1)^{-s}, \quad (u,v) \in S_n \times S_{n+1}.$$

Denote the corresponding Hamiltonian by $\mathbf{H}_{q,s}$.

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Theorem 7 (AK–Nicolussi)

Let $\mathcal{G} = \mathcal{A}_{q,s}$. Then:

(i)

$$\lambda_0(\mathbf{H}_{q,s}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}_{q,s}) = 0$$

if and only if $s \in [0,1)$.

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Notice that $\mathrm{K}_n \to 0$ as $n \to \infty$.

Theorem 7 (AK–Nicolussi)

Let $\mathcal{G} = \mathcal{A}_{q,s}$. Then:

(i)

$$\lambda_0(\mathbf{H}_{q,s}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}_{q,s}) = 0$$

if and only if $s \in [0,1)$.

(ii) If $s \ge 1$, then the operator $\mathbf{H}_{q,s}$ is uniformly positive and

$$\frac{1}{4} \le \lambda_0(\mathbf{H}_{q,s}) \le \pi^2, \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}_{q,s}) = \begin{cases} q^2, & s = 1, \\ +\infty, & s > 1. \end{cases}$$

Further examples

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Cayley graphs of finitely generated (infinite) groups.

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Locally finite tilings in the plane (in progress...)

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P. Exner, A. Kostenko, M. Malamud, and H. Neidhardt, *Spectral theory of infinite quantum graphs*, preprint, arXiv:1705.01831 (2017).

A. Kostenko and N. Nicolussi, *Spectral estimates for infinite quantum graphs*, preprint, arXiv:1711.02428 (2017).

Thank you for your attention!