

On the negative spectrum of quantum graphs

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based on a joint work with
Robert Schrader (Berlin)

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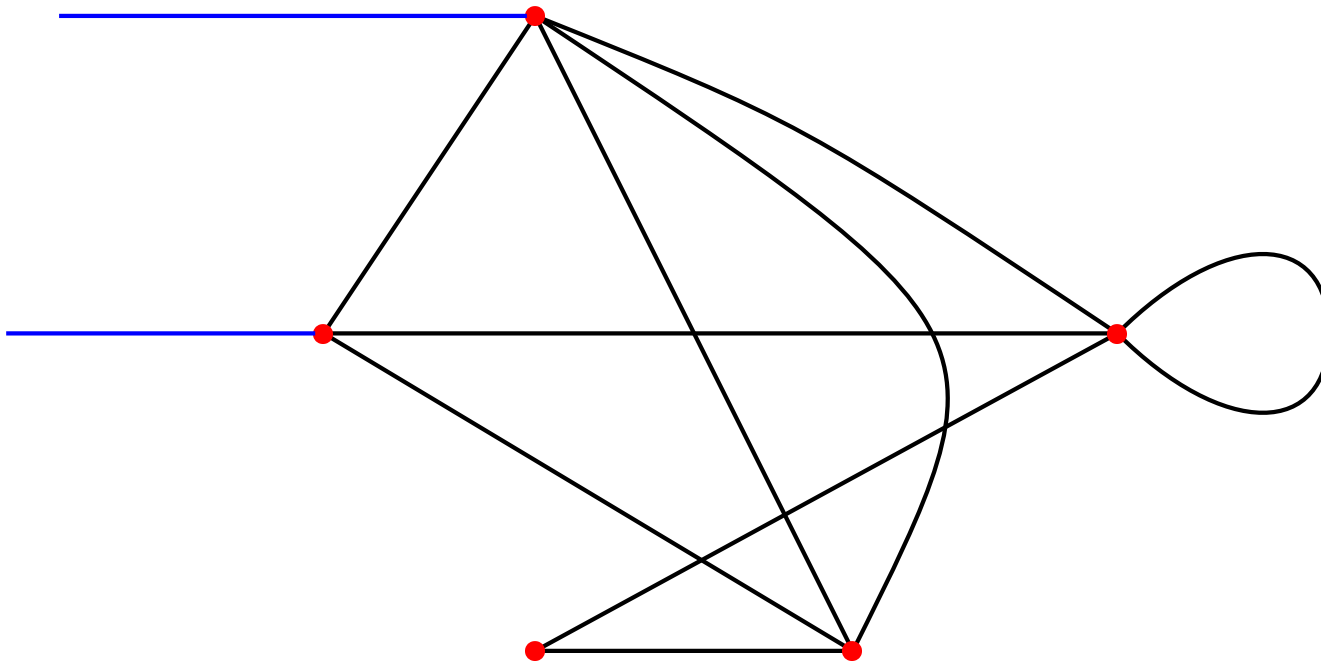
Self-Adjoint Laplace Operators

Number of Negative Eigenvalues

Lower Bounds on the Spectrum

Multiplicity of the Lowest Eigenvalue

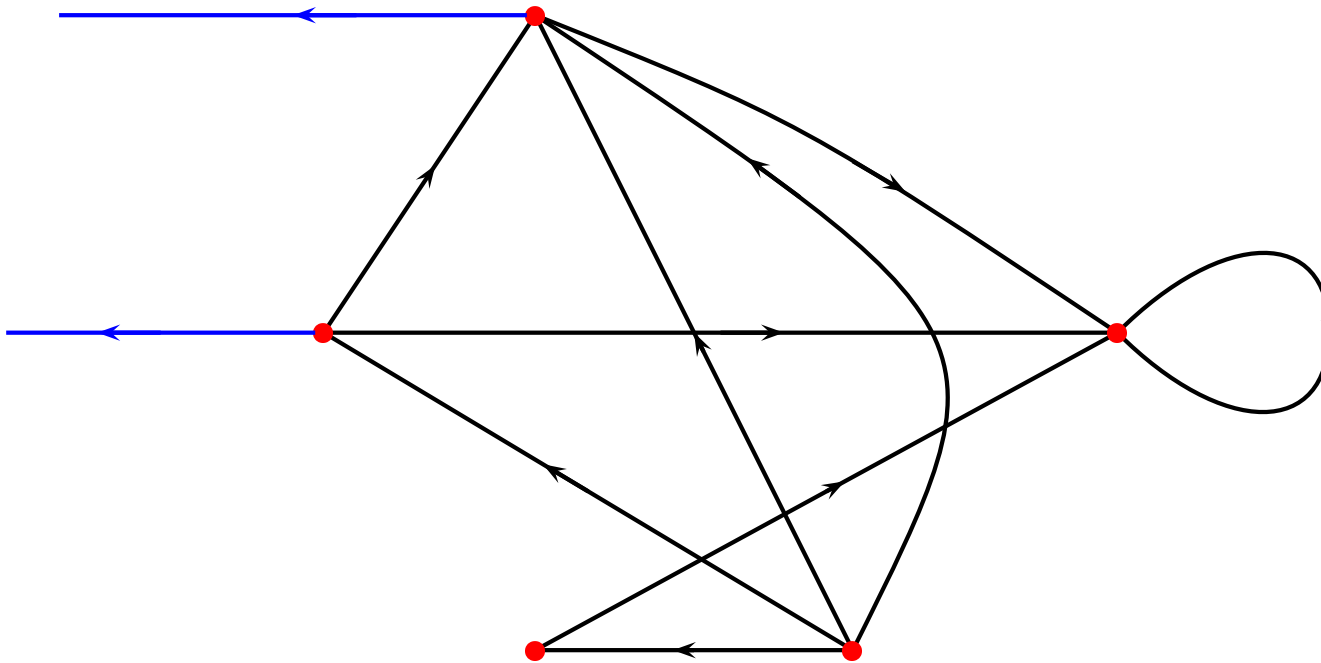
Let $G = (V, E)$ be a connected graph,
multiple edges and loops are allowed:



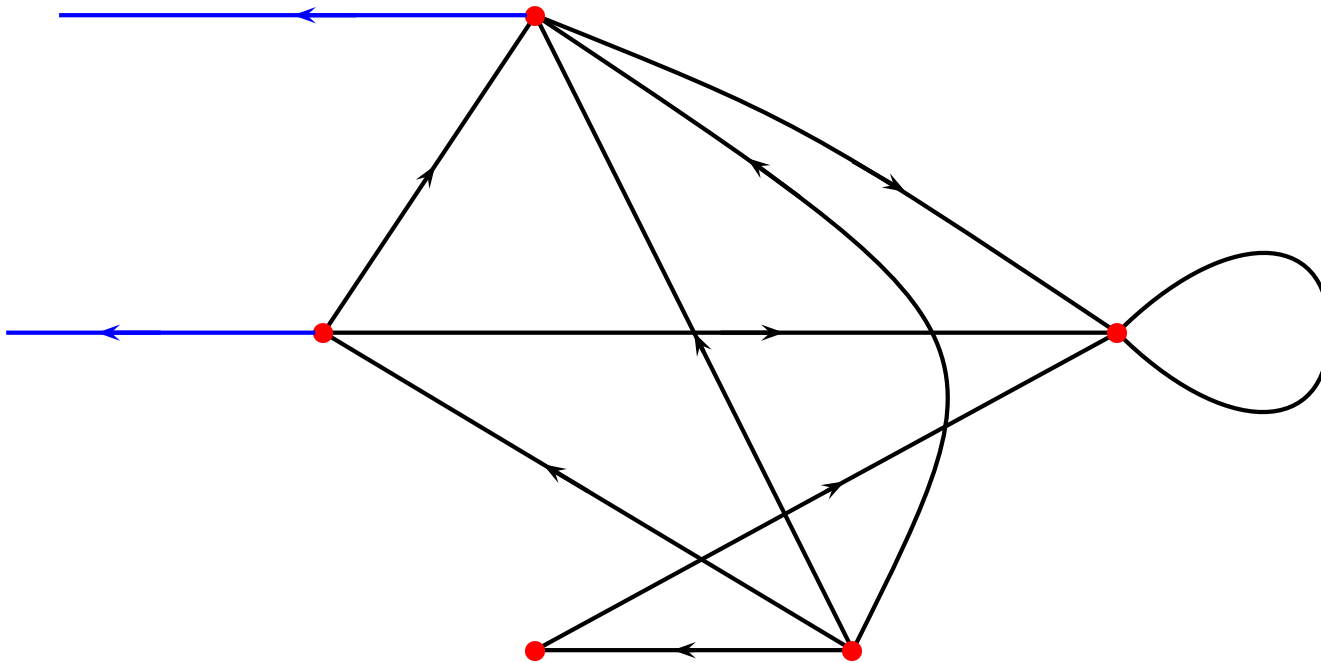
V vertex set

$E = E_{\text{int}} \cup E_{\text{ext}}$ edge set

Consider G as a directed graph:



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Each internal edge $j \in E_{\text{int}}$ will be associated with a bounded open interval $I_j := (0, a_j)$, $a_j > 0$, according to its orientation.

Each **external edge** $j \in E_{\text{ext}}$ will be associated with the semiline $I_j := (0, \infty)$.

Laplace Operators on Metric Graphs

- The Hilbert space

$$\mathcal{H} = \bigoplus_{j \in E} L^2(I_j) = \bigoplus_{j \in E_{\text{int}}} L^2((0, a_j)) \oplus \bigoplus_{j \in E_{\text{ext}}} L^2((0, \infty))$$

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- $\psi \in \mathcal{H} \iff \{\psi_j\}_{j \in E}$ with $\psi_j \in L^2(I_j)$ for $j \in E$

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■ $\psi \in \mathcal{H} \iff \{\psi_j\}_{j \in E}$ with $\psi_j \in L^2(I_j)$ for $j \in E$

■ For an arbitrary $\psi \in \mathcal{H}$ with $\psi_j \in H^2(I_j)$ (Sobolev space) set

$$\underline{\psi} = \begin{pmatrix} \{\psi_j(0)\}_{j \in E_{\text{ext}}} \\ \{\psi_j(0)\}_{j \in E_{\text{int}}} \\ \{\psi_j(a_j)\}_{j \in E_{\text{int}}} \end{pmatrix} \in \mathcal{K}, \quad \underline{\psi}' = \begin{pmatrix} \{\psi'_j(0)\}_{j \in E_{\text{ext}}} \\ \{\psi'_j(0)\}_{j \in E_{\text{int}}} \\ \{-\psi'_j(a_j)\}_{j \in E_{\text{int}}} \end{pmatrix} \in \mathcal{K} \cong \mathbb{C}^{2|E_{\text{int}}| + |E_{\text{ext}}|}$$

and $[\psi] := \begin{pmatrix} \psi \\ \psi' \end{pmatrix} \in \mathcal{K}_d := \mathcal{K} \oplus \mathcal{K}$ (space of boundary values).

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■ Let Δ_0 be the Laplace operator in \mathcal{H} defined on Sobolev functions in H^2 with the boundary conditions $[\psi] = 0$. It is a symmetric, closed, densely defined operator.

Self-Adjoint Laplace Operators

Theorem. The operator Δ with domain $\text{Dom}(\Delta)$ is a self-adjoint extension of the symmetric operator Δ_0 if and only if the subspace

$$\mathcal{M} := \{[\psi] \mid \psi \in \text{Dom}(\Delta)\} \subset \mathcal{K}_d$$

is **maximal isotropic** (= complex Lagrange plane), that is, the Hermitian symplectic form

$$\omega([\varphi], [\psi]) := \langle [\varphi], \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} [\psi] \rangle_{\mathbb{C}}, \quad \omega([\varphi], [\psi]) = -\overline{\omega([\psi], [\varphi])}$$

vanishes on \mathcal{M} and \mathcal{M} has a maximal dimension ($= |E_{\text{ext}}| + 2|E_{\text{int}}|$). We will write $\Delta(\mathcal{M})$ for the corresponding extension.

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Similar to the real symplectic theory, \mathcal{M} is maximal isotropic if and only if \mathcal{M}^{\perp} is maximal isotropic. Therefore, there is a duality transformation $\Delta(\mathcal{M}) \mapsto \Delta(\mathcal{M}^{\perp})$. Under this transformation $\Delta_{\text{Dirichlet}} \mapsto \Delta_{\text{Neumann}}$ and $\Delta_{\text{Neumann}} \mapsto \Delta_{\text{Dirichlet}}$.

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A subspace $\mathcal{M} \subset \mathcal{K}_d$ is maximal isotropic if and only if there are linear maps $A : \mathcal{K} \rightarrow \mathcal{K}$, $B : \mathcal{K} \rightarrow \mathcal{K}$ such that $(A \ B) : \mathcal{K}_d \rightarrow \mathcal{K}$ has maximal rank and AB^* is self-adjoint. Then

$$\mathcal{M} = \mathcal{M}(A, B) := \left\{ [\underline{\psi}] = \begin{pmatrix} \underline{\psi} \\ \underline{\psi}' \end{pmatrix} \mid A\underline{\psi} + B\underline{\psi}' = 0 \right\}$$

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Remarks:

- A and B define the boundary conditions

$$[\psi] \in \mathcal{M}(A, B) \iff A\underline{\psi} + B\underline{\psi}' = 0.$$

- $\mathcal{M}(A, B) = \mathcal{M}(TA, TB)$ for any invertible T .

Theorem [V.K., Schrader (1999), (2000); Harmer (2000)]. *The following statements are equivalent:*

- *The Laplace operator $\Delta(A, B)$ is self-adjoint,*
- *$(A \ B)$ has maximal rank and $AB^* = BA^*$,*
- *$S(k; A, B) := -(A + ikB)^{-1}(A - ikB)$ is unitary for some (and hence for all) $k > 0$.*

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$$S(k; A, B) = [(k - k_0)S(k_0; A, B) + (k + k_0)]^{-1} [(k + k_0)S(k_0; A, B) + (k - k_0)]$$

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Remarks:

- Any unitary S defines a self-adjoint Laplace operator $\Delta(A, B)$ with
$$A = -\frac{1}{2}(S - I), \quad B = \frac{1}{2i}(S + I).$$

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- Cut all internal edges of the graph and replace each of them by an external edge. $S(k; A, B)$ is the scattering matrix for the resulting completely disjoint graph.

Self-Adjoint Laplace Operators: Resolvent

The resolvent $(-\Delta(\mathcal{M}) - k^2)^{-1}$ is the integral operator with the $(|E_{\text{int}}| + |E_{\text{ext}}|) \times (|E_{\text{int}}| + |E_{\text{ext}}|)$ matrix-valued integral kernel given by

$$r_{\mathcal{M}}(x, y; k) = r^{(0)}(x, y, k) + \frac{i}{2k} \Phi(x, k) R_+(k)^{-1} [I - S(k; \mathcal{M}) T(k)]^{-1} S(k; \mathcal{M}) R_+(k)^{-1} \Phi(y, k)^T,$$

where $\Phi(x, k) := \begin{pmatrix} \phi(x; k) & 0 & 0 \\ 0 & \phi_+(x; k) & \phi_-(x; k) \end{pmatrix},$

$$R_+(k) := \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & e^{-ika} \end{pmatrix}, \quad T(k) := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & e^{ika} \\ 0 & e^{ika} & 0 \end{pmatrix},$$

with diagonal matrices $\phi(x; k) = \text{diag}\{e^{ikx_j}\}_{j \in E_{\text{ext}}}$, $\phi_{\pm}(x; k) = \text{diag}\{e^{\pm ikx_j}\}_{j \in E_{\text{int}}}$, and

$$e^{ika} = \text{diag}\{e^{\pm ika_j}\}_{j \in E_{\text{int}}}, \quad [r^{(0)}(x, y, k)]_{j, j'} = i\delta_{j, j'} \frac{e^{ik|x_j - y_j|}}{2k}, \quad x_j, y_j \in I_j.$$

Self-Adjoint Laplace Operators

Assume:

[Kuchment (2004)]

P an orthogonal projection (possibly zero),
 L self-adjoint operator such that $LP^\perp = 0$.

Set $A = P^\perp + L$, $B = P$. Then $AB^* = L$ and $(A \ B)$ has maximal rank. Hence, $\mathcal{M}(A, B)$ is maximal isotropic.

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Do we get all the maximal isotropic subspaces? Yes! Take an arbitrary unitary S_0 . Split off its eigensubspace corresponding to the eigenvalue -1 . Denote by \widehat{S}_0 the restriction of S onto the complementary subspace. Take its Cayley transform $\widehat{L} = i(I + \widehat{S}_0)^{-1}(I - \widehat{S}_0)$. Let L be the extension of \widehat{L} to the whole of \mathcal{K} . Then we obtain

$$S(1; P^\perp + L, P) = -(P^\perp + L + iP)^{-1}(P^\perp + L - iP) = S_0,$$

where P is the orthogonal projection onto the eigensubspace of S_0 corresponding to the eigenvalue -1 .

Self-Adjoint Laplace Operators

For any maximal isotropic subspace \mathcal{M} there are unique $P_{\mathcal{M}}$ and $L_{\mathcal{M}}$ such that

$$\mathcal{M} = \left\{ [\underline{\Psi}] = \begin{pmatrix} \underline{\Psi} \\ \underline{\Psi}' \end{pmatrix} \mid (P^{\perp} + L)\underline{\Psi} + P\underline{\Psi}' = 0 \right\}.$$

What happens with $L_{\mathcal{M}}$ under the duality transformation $\mathcal{M} \mapsto \mathcal{M}^{\perp}$?

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Claim: $L_{\mathcal{M}^{\perp}} = -L_{\mathcal{M}}$.

We know that $\mathcal{M}(A, B)^{\perp} = \mathcal{M}(-B, A)$. Hence, the duality transformation sends AB^* to $(-B)A^* = -BA^* = -AB^*$.

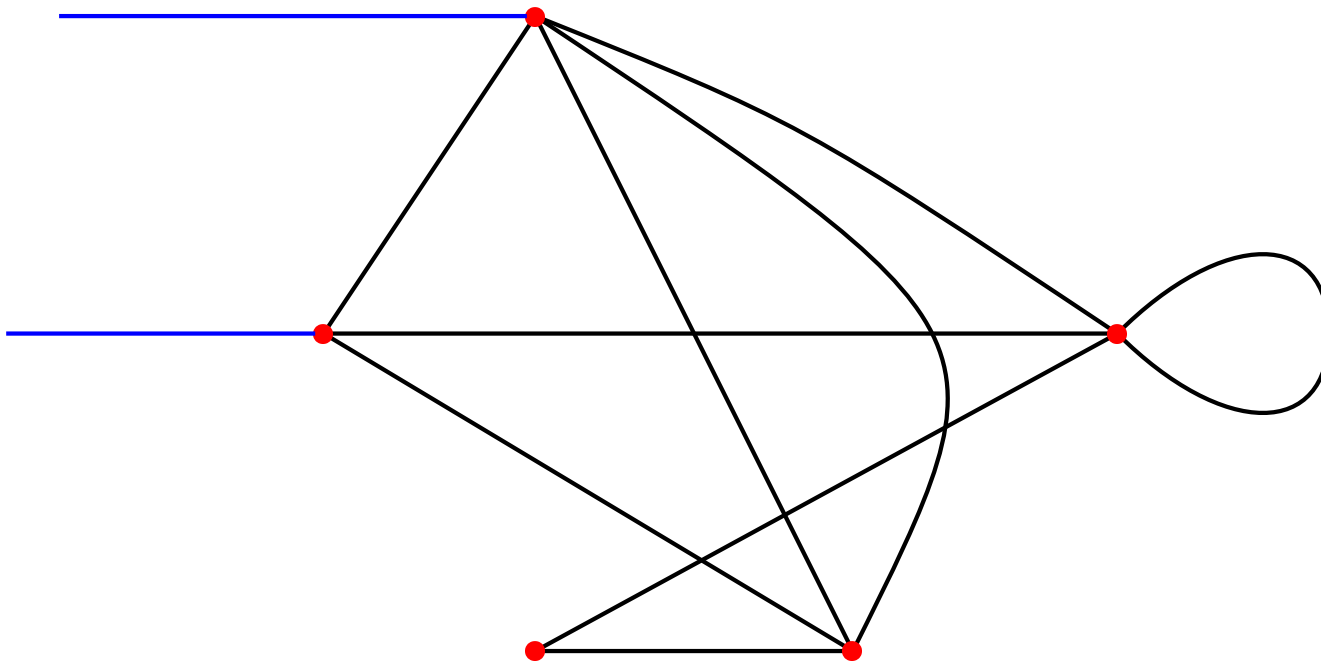
Take

$$A = P_{\mathcal{M}}^{\perp} + L_{\mathcal{M}}, \quad B = P_{\mathcal{M}} \quad \Rightarrow \quad AB^* = L_{\mathcal{M}}.$$

Thus, the duality transformation sends $L_{\mathcal{M}}$ to $-L_{\mathcal{M}}$.

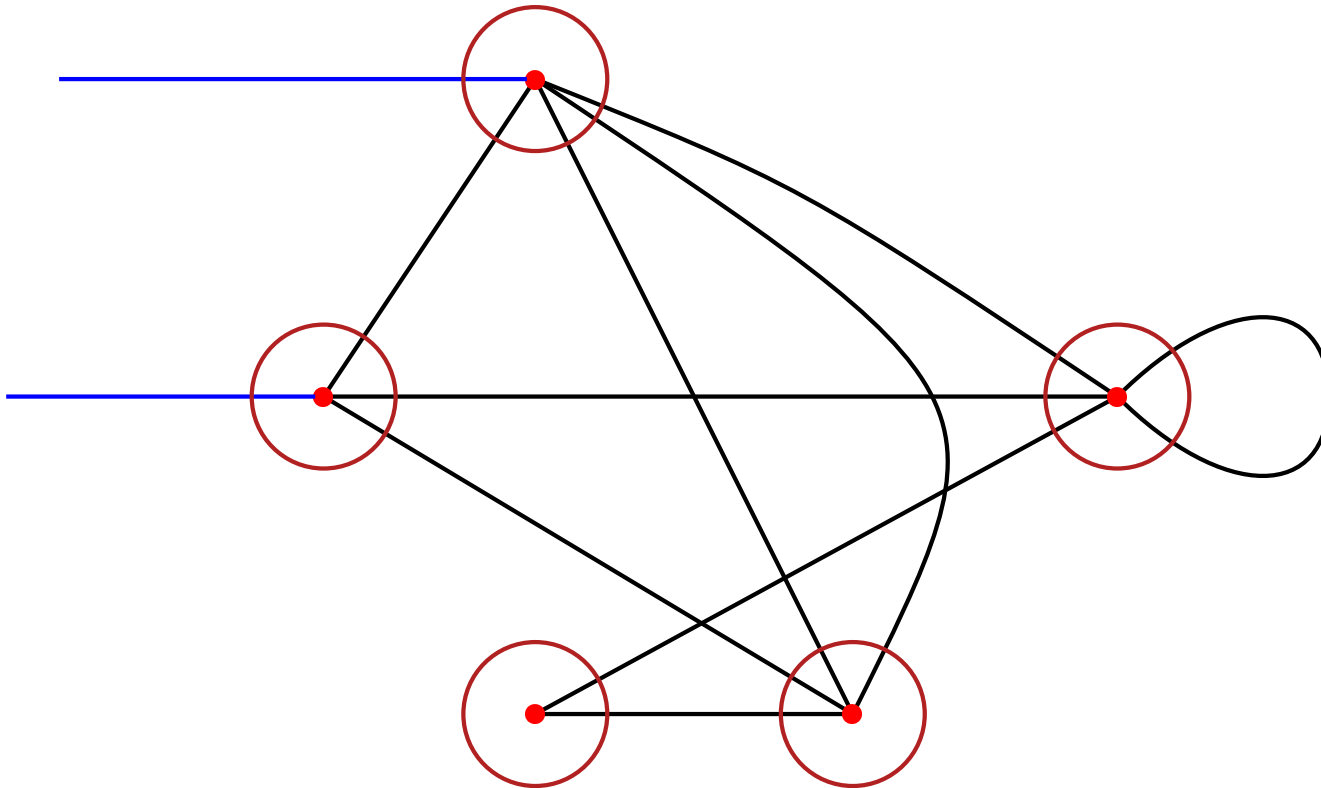
Local Boundary Conditions

The boundary conditions are **local**, if $S(k; \mathcal{M})$ can be written in the block diagonal form $S(k; \mathcal{M}) = \bigoplus_{v \in V} S(k; \mathcal{M}_v)$ such that each block corresponds to a particular vertex.



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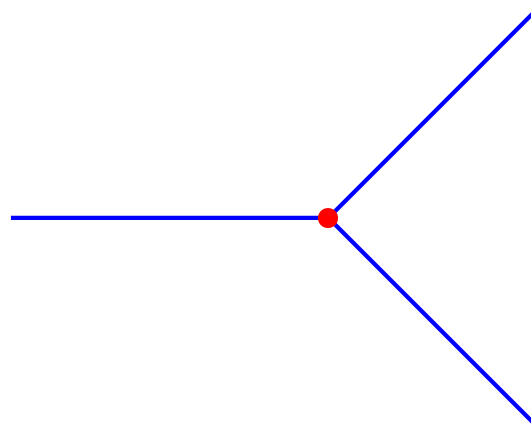
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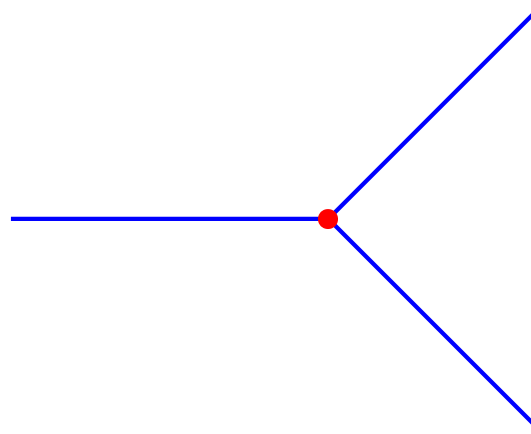
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Let G be a “star graph”, that is a graph with a single vertex and no internal edges:



Claim: The number of negative eigenvalues of $-\Delta(A, B)$ (counting multiplicity) equals the number of positive eigenvalues of AB^* (counting multiplicity).

Remark: By Sylvester’s Inertia Law the number of positive eigenvalues of $(TA)(TB)^* = TAB^*T^*$ does not depend on T whenever T is invertible. Thus, AB^* and L have an equal number of positive eigenvalues.

Number of Negative Eigenvalues

Proof of $N_-(-\Delta(A, B)) = N_+(AB^*)$: With the ansatz $\psi_j(x) = \chi_j e^{-\varkappa x}$ we obtain that ψ is an eigenfunction of $-\Delta(A, B)$ with the eigenvalue $-\varkappa^2 < 0$ if and only if

$$(A - \varkappa B)\chi = 0.$$

The number of negative eigenvalues of $-\Delta(A, B)$ equals the number of positive zeroes of the function

$$\begin{aligned} f(\varkappa) &:= \det(A - \varkappa B) = \det(T(P^\perp + L - \varkappa P)) \\ &= \det T \det(P^\perp + L - \varkappa P) = \det T \det \begin{pmatrix} P^\perp & 0 \\ 0 & PLP - \varkappa P \end{pmatrix} \\ &= \det T \det(L - \varkappa). \end{aligned}$$

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For arbitrary graphs we have the inequality $N_-(-\Delta(A, B)) \leq N_+(AB^*)$.

A weaker statement: If $AB^* \leq 0$, then $-\Delta(A, B) \geq 0$.

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Proof: Compute the quadratic form of $-\Delta(A, B)$:

$$\langle \psi, -\Delta(A, B)\psi \rangle_{\mathcal{H}} = \sum_{j \in \mathcal{E}} \langle \psi'_j, \psi'_j \rangle_{L^2(I_j)} + \langle [\Psi], Q[\Psi] \rangle_{\mathcal{K}_d}, \quad [\Psi] := \begin{pmatrix} \Psi \\ \underline{\psi'} \end{pmatrix},$$

where

$$Q = \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \quad \text{with respect to the orthogonal decomposition} \quad \mathcal{K}_d = \mathcal{K} \oplus \mathcal{K}.$$

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It is straightforward to verify that

$$P_{\mathcal{M}} = \begin{pmatrix} -B^* \\ A^* \end{pmatrix} (AA^* + BB^*)^{-1} \begin{pmatrix} -B & A \end{pmatrix}$$

is the orthogonal projection onto $\mathcal{M} = \left\{ [\Psi] = \begin{pmatrix} \underline{\Psi} \\ \underline{\Psi}' \end{pmatrix} \mid A\underline{\Psi} + B\underline{\Psi}' = 0 \right\}$.

Since $\psi \in \mathcal{H}$ belongs to the domain of $-\Delta(A, B)$, we have $P_{\mathcal{M}}[\psi] = [\psi]$. Therefore,

$$\langle [\psi], Q[\psi] \rangle_{\mathcal{K}_d} = \langle [\psi], P_{\mathcal{M}} Q P_{\mathcal{M}} [\psi] \rangle_{\mathcal{K}_d}$$

with

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Putting all together we obtain

$$\langle \psi, -\Delta(A, B)\psi \rangle_{\mathcal{H}} = \sum_{j \in \mathcal{E}} \langle \psi'_j, \psi'_j \rangle_{L^2(I_j)} + \langle [\psi], P_{\mathcal{M}} Q P_{\mathcal{M}} [\psi] \rangle_{\mathcal{K}_d} \geq 0.$$

□

A Special Class of Positive Operators

Let $\mathcal{M} = \mathcal{M}(A, B)$ be a maximal isotropic subspace. The following conditions are equivalent:

- $S(k; \mathcal{M})$ is k -independent,
- $S(k; \mathcal{M})$ is self-adjoint for some $k > 0$,
- $S(k; \mathcal{M})^2 = I$ for some $k > 0$,
- $AB^* = 0$.

If $S(k; \mathcal{M})$ is k -independent, then $S(k; \mathcal{M}^\perp) = -S(k; \mathcal{M})$ is k -independent, too.

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Examples:

- Dirichlet $S(\mathcal{M}_D) = -I$ and Neumann $S(\mathcal{M}_N) = I$,
- “standard” $[S(\mathcal{M}_{\text{st}})]_{j,j'} = \frac{2}{\deg(v)} - \delta_{j,j'}$ and
“co-standard” $[S(\mathcal{M}_{\text{st}}^\perp)]_{j,j'} = -\frac{2}{\deg(v)} + \delta_{j,j'}$,
- all magnetic perturbations of the standard boundary conditions $U^* S(\mathcal{M}_{\text{st}}) U$,
 U depends on magnetic fluxes.

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- $S(k; \mathcal{M})$ is k -independent,
- $S(k; \mathcal{M})$ is self-adjoint for some $k > 0$,
- $S(k; \mathcal{M})^2 = I$ for some $k > 0$,
- $AB^* = 0$.

If $S(k; \mathcal{M})$ is k -independent, then $S(k; \mathcal{M}^\perp) = -S(k; \mathcal{M})$ is k -independent, too.

Examples:

- Dirichlet $S(\mathcal{M}_D) = -I$ and Neumann $S(\mathcal{M}_N) = I$,
- “standard” $[S(\mathcal{M}_{\text{st}})]_{j,j'} = \frac{2}{\deg(v)} - \delta_{j,j'}$ and
“co-standard” $[S(\mathcal{M}_{\text{st}}^\perp)]_{j,j'} = -\frac{2}{\deg(v)} + \delta_{j,j'}$,
- all magnetic perturbations of the standard boundary conditions $U^* S(\mathcal{M}_{\text{st}}) U$,
 U depends on magnetic fluxes.

Remark: Standard and Dirichlet are the only two boundary conditions with the property that all functions in $\text{Dom}(\Delta(\mathcal{M}))$ are continuous.

Theorem [V.K., Potthoff, Schrader (in preparation)]. *The following statements are equivalent:*

- *The Laplace operator $-\Delta(A, B)$ is **m-accretive**, that is,*

$$\operatorname{Re}\langle \psi, -\Delta(A, B)\psi \rangle \geq 0 \quad \text{for all} \quad \psi \in \operatorname{Dom}(-\Delta(A, B)),$$

- *$(A \ B)$ has maximal rank and $\operatorname{Re}AB^* \leq 0$,*
- *$S(i\kappa; A, B) := -(A - \kappa B)^{-1}(A + \kappa B)$ is contractive for some (and hence for all) $\kappa > 0$.*

A Generalization of Positivity

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- *$S(i\kappa; A, B) := -(A - \kappa B)^{-1}(A + \kappa B)$ is contractive for some (and hence for all) $\kappa > 0$.*

The following statements are equivalent:

- *The Laplace operator $-\Delta(A, B)$ is ***m-dissipative***, that is,*

$$\operatorname{Im}\langle \psi, -\Delta(A, B)\psi \rangle \geq 0 \quad \text{for all} \quad \psi \in \operatorname{Dom}(-\Delta(A, B)),$$

- *$(A \ B)$ has maximal rank and $\operatorname{Im}AB^* \leq 0$,*
- *$S(-k; A, B) := -(A - ikB)^{-1}(A + ikB)$ is contractive for some (and hence for all) $k > 0$.*

Lower Bounds on the Spectrum

Self-Adjoint Laplace
Operators

Number of Negative
Eigenvalues

Lower Bounds on the
Spectrum

Multiplicity of the Lowest
Eigenvalue

- For star graphs $\lambda_{\min} = -\|L_+\|^2$, its multiplicity equal to the multiplicity of the largest eigenvalue of L . It is a square of the biggest positive solution of the equation

$$\det(A - \kappa B) = 0.$$

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- For general graphs the situation is much more interesting. Peter Kuchment (2004) proved the following bound:

$$\lambda_{\min} \geq -4\|L\|(|E_{\text{ext}}| + 2|E_{\text{int}}|) \max \left\{ 2\|L\|, \max_{i \in E_{\text{int}}} \frac{1}{a_i} \right\},$$

For large graphs the right hand side goes to $-\infty$.

Lower Bounds on the Spectrum

Theorem [V.K., Schrader (2006)]. Assume that $E_{\text{int}} \neq \emptyset$. Then

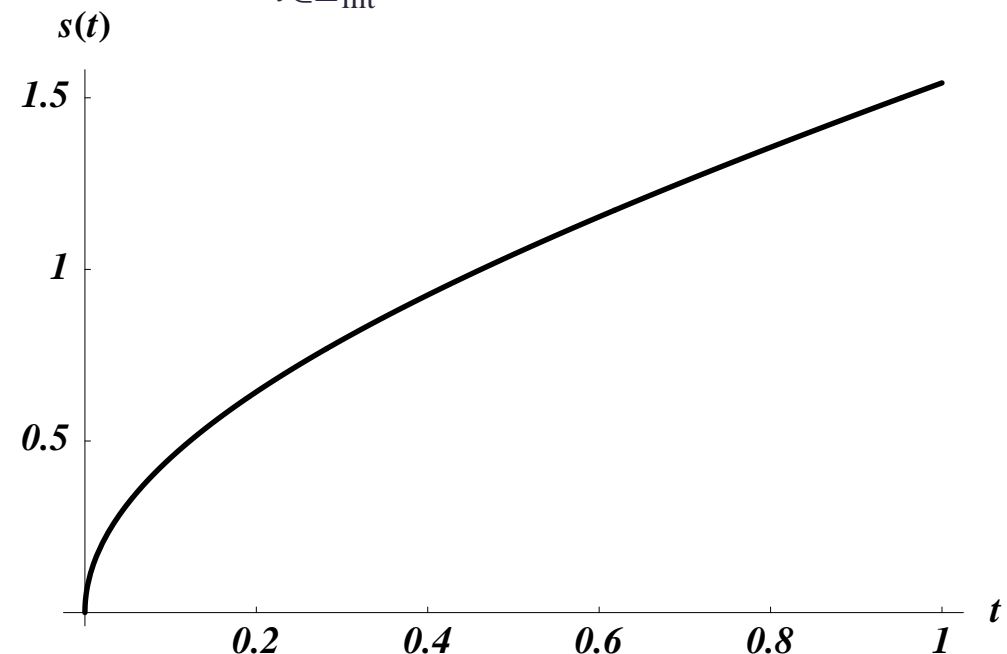
$$\lambda_{\min} \geq -s_a(\|L_+\|)^2,$$

where L_+ denotes the positive part of the operator L and $s_a(t)$ is the unique nonnegative solution of the equation

$$s \cdot \tanh\left(\frac{as}{2}\right) = t, \quad a := \min_{i \in E_{\text{int}}} a_i.$$

Properties of $s_a(t)$:

- $s_a(0) = 0$,
- $s_a(t) \sim t$ for $t \rightarrow \infty$,
- $s_a(t) \sim \sqrt{\frac{2t}{a}}$ for $a \rightarrow 0$.



Lower Bounds on the Spectrum: An Example

Does $s_a(t) \sim \sqrt{\frac{2t}{a}}$ for $a \rightarrow 0$ corresponds to the correct behaviour of the lowest eigenvalue?

Example: Consider the operator

$$H_n = -\frac{d^2}{dx^2} - \sum_{k=1}^n \delta(x - 1/k), \quad \varkappa \psi(0) + \psi'(0) = 0, \quad \varkappa > 0 \quad \text{on} \quad L^2(0, \infty).$$



For $\psi(x) := \sqrt{2\varkappa}e^{-\varkappa x}$ compute the quadratic form

$$\langle \psi, H_n \psi \rangle = \int_0^\infty \psi'(x)^2 dx - \sum_{k=1}^n \psi(1/k)^2 = \varkappa^2 - 2\varkappa \sum_{k=1}^n e^{-2\varkappa/k}.$$

For $n \rightarrow \infty$ the sum goes to $+\infty$. Thus, $\lambda_{\min}(H_n) \xrightarrow{n \rightarrow \infty} -\infty$.

Lower Bounds on the Spectrum

Proof of $\lambda_{\min} \geq -s_a(\|L_+\|)^2$. Let $\varkappa_0 > 0$ be the biggest solution of the equation $\det(A - \varkappa B) = 0$. Obviously,

$$\varkappa_0 := \|L_+\| = \text{the biggest positive eigenvalue of } L$$

Estimate

$$\|S(i\varkappa; A, B)\| = \left\| -P_{\text{Ker}B} - P_{\text{Ker}B}^\perp \frac{L + \varkappa}{L - \varkappa} P_{\text{Ker}B}^\perp \right\| = \frac{\varkappa + \varkappa_0}{\varkappa - \varkappa_0} > 1$$

for all $\varkappa > \varkappa_0$.

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for all $\varkappa > \varkappa_0$. The number $-\varkappa_+^2$ is the lowest eigenvalue of $-\Delta(A, B)$ if \varkappa_+ is the biggest solution of the equation

$$\det[I - S(i\varkappa; A, B)T(i\varkappa)] = 0 \quad \text{with} \quad T(i\varkappa) := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & e^{-\varkappa \underline{a}} \\ 0 & e^{-\varkappa \underline{a}} & 0 \end{pmatrix}$$

with $e^{-\varkappa \underline{a}} := \text{diag}(e^{-\varkappa a_j})_{j \in E_{\text{int}}}$.

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with $e^{-\varkappa \underline{a}} := \text{diag}(e^{-\varkappa a_j})_{j \in E_{\text{int}}}$. Therefore,

$$\|S(i\varkappa_+; A, B)T(i\varkappa_+)\| \geq 1$$

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with $e^{-\varkappa \underline{a}} := \text{diag}(e^{-\varkappa a_j})_{j \in E_{\text{int}}}$. Therefore,

$$\|S(i\varkappa_+; A, B)T(i\varkappa_+)\| \geq 1 \Rightarrow \|S(i\varkappa_+; A, B)\| \|T(i\varkappa_+)\| \geq 1.$$

Lower Bounds on the Spectrum: The Proof

Thus,

$$\varkappa_+ < \varkappa_1 := \inf\{\varkappa > \varkappa_0 \mid \|S(i\varkappa; A, B)\| \|T(i\varkappa)\| < 1\}.$$

Since

$$\|S(i\varkappa; A, B)\| \|T(i\varkappa)\| = \frac{\varkappa + \varkappa_0}{\varkappa - \varkappa_0} e^{-a\varkappa} \quad \text{for all } \varkappa > \varkappa_0,$$

\varkappa_1 is not larger than the unique positive solution of the equation

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Thus,

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\varkappa_1 is not larger than the unique positive solution of the equation

$$\frac{\varkappa + \varkappa_0}{\varkappa - \varkappa_0} e^{-a\varkappa} = 1 \quad \Leftrightarrow \quad \varkappa = s_a(\varkappa_0).$$

We are done!

Lower Bounds on the Spectrum: A Remark

Consider an arbitrary finite graph. Keep all but one edge length (say a_0) fixed and let $a_0 \rightarrow 0$. Then $a := \min_{i \in E_{\text{int}}} a_i \rightarrow 0$, but the lowest eigenvalue remains finite. The bound

$$\lambda_{\min} \geq -s_a(\|L_+\|)^2,$$

becomes meaningless in this limit:

$$\lambda_{\min} \geq -\lim_{a_0 \rightarrow 0} s_a(\|L_+\|)^2 = -\infty.$$

Quite unsatisfactory!

Multiplicity of the Lowest Eigenvalue

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Assume that the boundary conditions are local, that is,

$S(k; \mathcal{M}) = \bigoplus_{v \in V} S(k; \mathcal{M}_v)$ such that each block corresponds to a particular

vertex. Assume, in addition,

$$I + S(i\kappa, \mathcal{M}_v) > 0 \quad (\text{componentwise})$$

for all vertices $v \in V$ and all sufficiently large $\kappa > 0$. Then the eigenvalue λ_{\min} is simple.

Proof is by using the semigroup technique.

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Thank You For Your Attention!

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