Relative monotonicity of secular determinants of quantum graphs

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Motivation

- Quantum graph provides useful models for complex systems in the fields of natural science, engineering and social sciences
- In the long term, our project is to find a more efficient algorithm of computing eigenvalues of quantum graphs
- we conjectured that the secular determinants of quantum graphs are relatively monotonic

Background

DEFINITION: Quantum graph Γ(V,E) ,where V is the set of vertices and E is the set of edges, is a metric graph equipped with a Hamiltonian operator H (1) , accompanied by "appropriate" vertex conditions (2).

- eigenvalue equation for the Schrödinger operator:

(1) $$-\frac{d^2 f}{dx^2} + V(x) \cdot f(x) = k^2 \cdot f(x)$$

- (2) Vertex conditions:
  - Neumann condition:

    $f(x)$ is continuous on Γ and at each vertex v one has $\sum_{e \in E_v} \frac{df}{dx_e}(v) = 0$

  - Dirichlet condition:

    $f(x)$ is continuous on Γ and $f(v) = 0$

A trivial example: interval

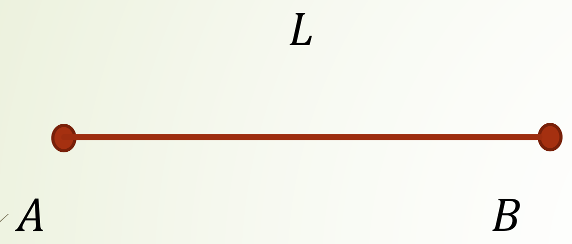


Figure 1. interval [0,L], Neumann condition on endpoints A,B, and 0 corresponding A ;

(1) $V(x) \equiv 0;$

Solution for $-f'' = k^2 f$ on L:

(2) $f(x) = C_1 \cos(kx) + C_2 \sin(kx)$

Apply vertex conditions:

(3) $f'(0) = 0$

(4) $-f'(L) = 0$

we can solve eigenvalues:

(5) $k^2 = (\frac{\pi n}{L})^2 \quad , n \in N$

Example: Lasso graph

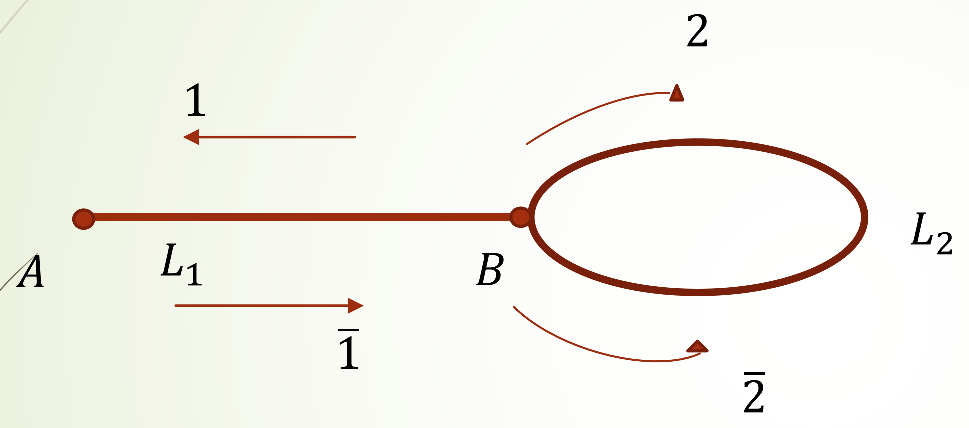


Figure 2. Γ(V,E) Lasso graph V={A,B} ; E={$[0, L_1], [0, L_2]$} where 0 corresponding connected point ; Neumann condition on vertices

Solution for $-f'' = k^2 f$ on L_1, L_2 :

(6) $f_1 = a_1 \cdot e^{ikx} + a_{\bar{1}} \cdot e^{ik(L_1 - x)}$

(7) $f_2 = a_2 \cdot e^{ikx} + a_{\bar{2}} \cdot e^{ik(L_2 - x)}$

Apply vertex condition:

(8) $-f_1'(L_1) = -ika_1 e^{ikL_1} + ika_{\bar{1}} = 0$

(9) $f_1'(0) + f_2'(0) - f_2'(L_2) = 0$

(10) $f_1(0) = f_2(0) = f_2(L_2)$

Example: Lasso graph

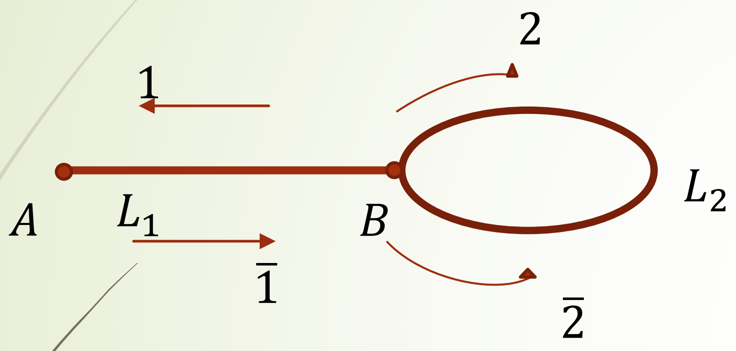


Figure 2. Γ(V,E) Lasso graph V={A,B} ; E={$[0, L_1], [0, L_2]$} where 0 corresponding connected point ; Neumann condition on vertices

We get the system

(11) $a_1 = -\frac{1}{3} a_{\bar{1}} e^{ikL_1} + \frac{2}{3} a_2 e^{ikL_2} + \frac{2}{3} a_{\bar{2}} e^{ikL_2}$

(12) $a_{\bar{1}} = a_1 e^{ikL_1}$

(13) $a_2 = \frac{2}{3} a_{\bar{1}} e^{ikL_1} + \frac{2}{3} a_2 e^{ikL_2} - \frac{1}{3} a_{\bar{2}} e^{ikL_2}$

(14) $a_{\bar{2}} = \frac{2}{3} a_{\bar{1}} e^{ikL_1} - \frac{1}{3} a_2 e^{ikL_2} + \frac{2}{3} a_{\bar{2}} e^{ikL_2}$

Example: Lasso graph

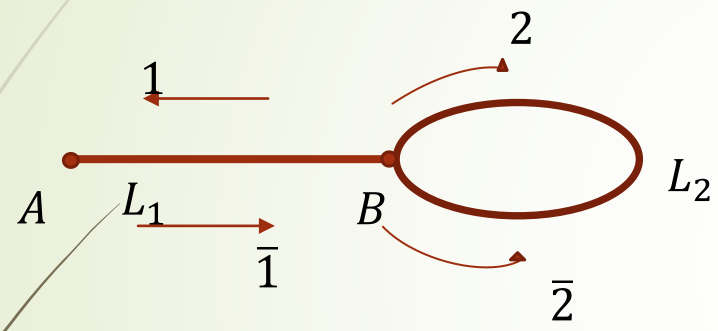


Figure 2. Γ(V,E) Lasso graph
V={A,B} ; E={$[0, L_1], [0, L_2]$}
where 0 corresponding connected point ; Neumann condition on vertices

The system can be written as:

(15)

$$\begin{bmatrix} a_1 \\ a_{\bar{1}} \\ a_2 \\ a_{\bar{2}} \end{bmatrix} = \begin{bmatrix} 0 & -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ 1 & 0 & 0 & 0 \\ 0 & \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \\ 0 & \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \end{bmatrix} \begin{bmatrix} e^{ikL_1} & 0 & 0 & 0 \\ 0 & e^{ikL_1} & 0 & 0 \\ 0 & 0 & e^{ikL_2} & 0 \\ 0 & 0 & 0 & e^{ikL_2} \end{bmatrix} \begin{bmatrix} a_1 \\ a_{\bar{1}} \\ a_2 \\ a_{\bar{2}} \end{bmatrix}$$

Notation:

S $\qquad$ $D(k)$

$k^2 (k \neq 0)$ is the eigenvalue of the graph iff $\mathbf{det(I - SD(k)) = 0}$, we call the determinant **secular determinant**.

Secular determinant (Neumann condition graph)

For the general Neumann condition graph Γ(V,E), first consider the single vertex in Γ(V,E), which has d edges attach to it. Denote the length of j-th edge is L_j,

the solution on j-th edge:

Figure 3. a vertex with Neumann condition c

(16) $$f_j = a_j \cdot e^{ikx} + a_{\bar{j}} \cdot e^{ik(L_j - x)}$$

Apply the vertex condition:

(17) $$\sum_{j=1}^{d} a_j - \sum_{j=1}^{d} a_{\bar{j}} e^{ikL_j} = 0$$

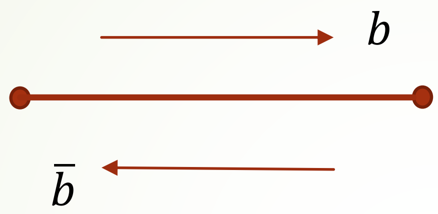
(18) $$a_j + a_{\bar{j}} e^{ikL_j} = a_l + a_{\bar{l}} e^{ikL_l} ,\quad \text{for } \forall l, k \in N^* \; and \; l, k \le d$$

By (16)&(17)&(18) we solving a_n for $1 \le n \le d$:

(19) $$a_n = -a_{\bar{n}} e^{ikL_n} + \frac{2}{d} \sum_{j=1}^{d} a_{\bar{j}} e^{ikL_j}$$

Secular determinant (Neumann condition graph)

Then we consider the whole graph $\Gamma(V,E)$



In the 2|E|-dimensional complex space, with dimensions indexed by the directed edges. we get $2|E| \times 2|E|$ matrix S and D(k)for $\Gamma(V,E)$:

(20) $$D(k)_{b,b} = e^{ikL_b}$$

(21) $$S_{b',b} = \begin{cases} \frac{2}{d} - 1 & \text{if } b' = \bar{b} \\ \frac{2}{d} & \text{if } b' \text{ follows } b \text{ and } b' \neq \bar{b} \\ 0 & \text{otherwise} \end{cases}$$

The secular determinant is $\mathbf{det}(\boldsymbol{I} - \boldsymbol{SD}(\boldsymbol{k}))$

Proposal

- Change a vertex condition (Neumann condition to Dirichlet condition)

  e.g.

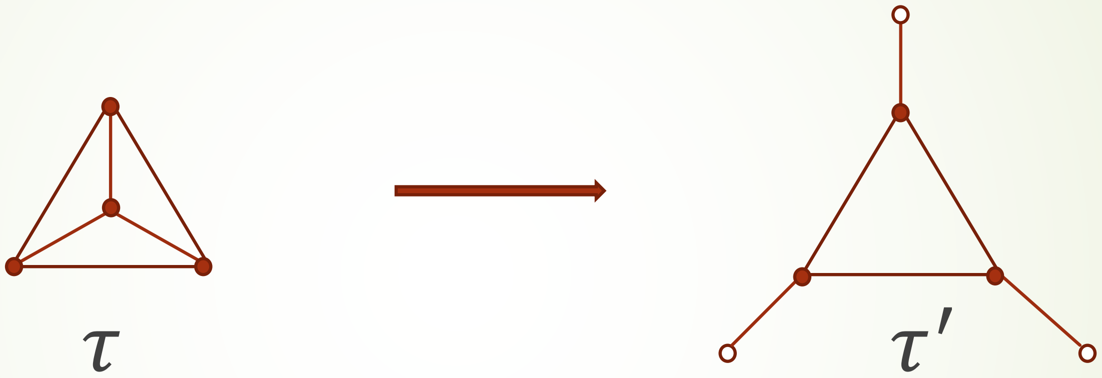


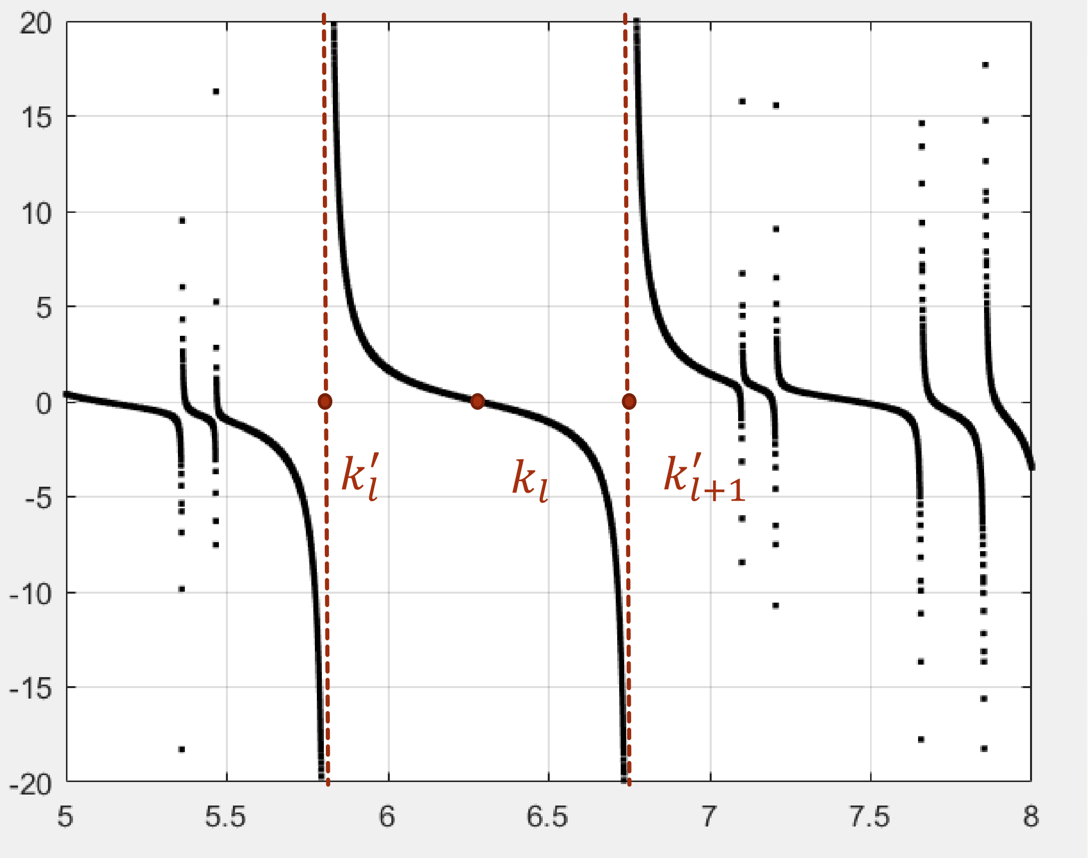
Figure 4.

Conjecture:

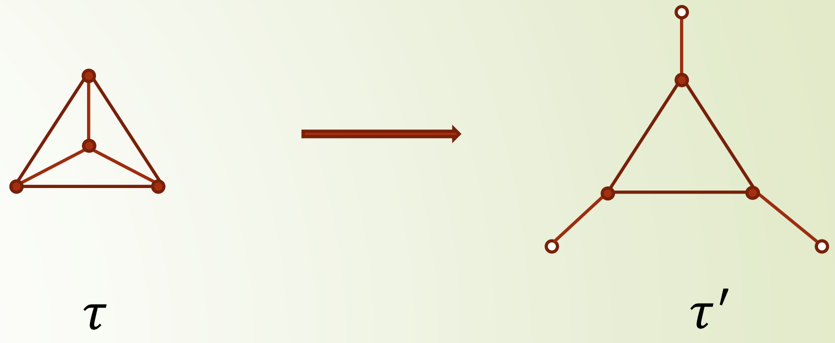
Define a quantum graph τ with Neumann condition on its vertices, obtained the quantum graph τ' by changing one of the vertices condition to Dirichlet condition. Define $f(k) = \frac{\det(I - S_\tau D_\tau(k))}{\det(I - S_{\tau'} D_{\tau'}(k))}$, and f(k) has negative derivatives except the location where k^2 is eigenvalue of τ'.

poles.

Application



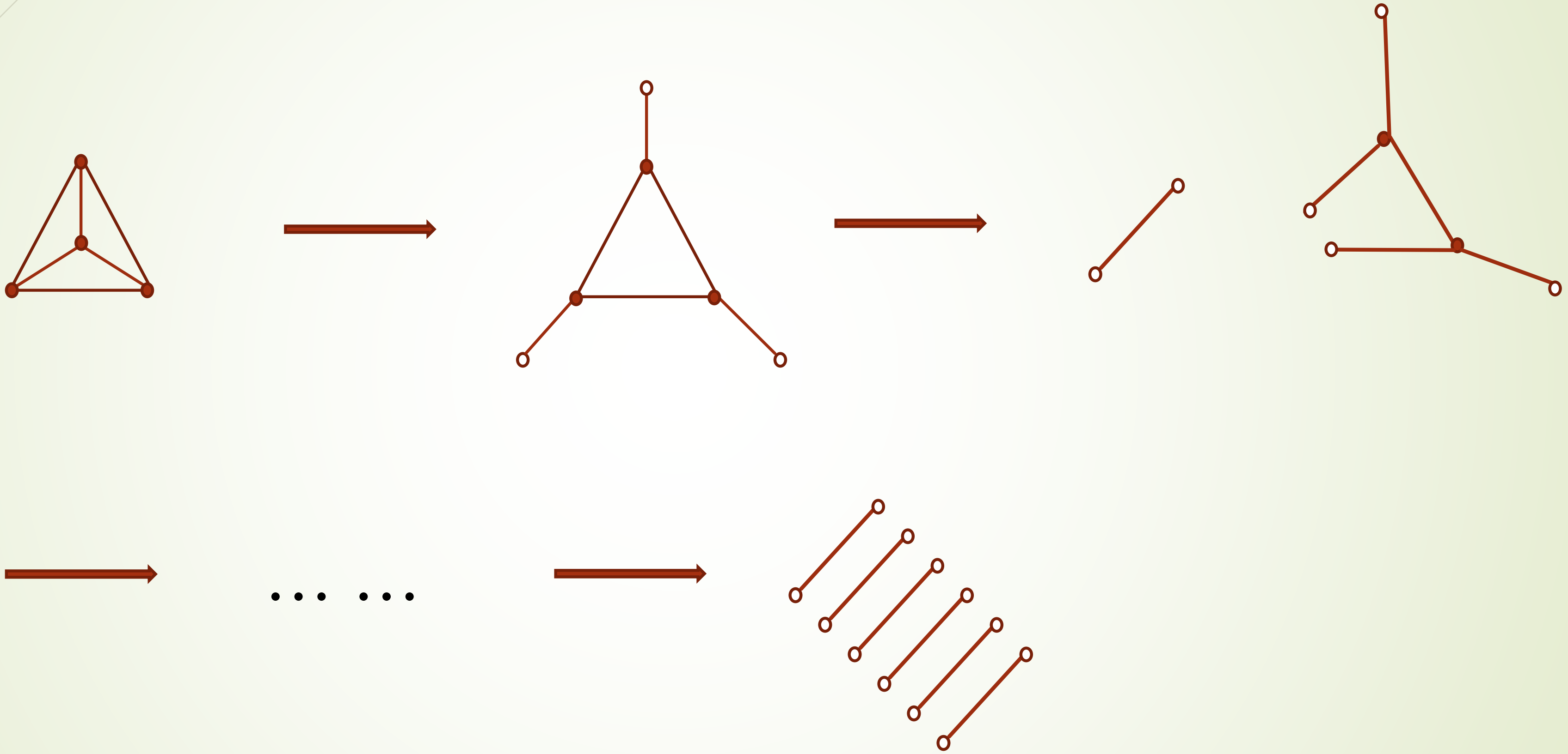
Graph 1. part of the graph for f(k)



$$f(k) = \frac{\det(I - S_\tau D_\tau(k))}{\det(I - S_{\tau'} D_{\tau'}(k))}$$

There is only one eigenvalue lies between two poles and the derivative is always negative. Using Secant Algorithm can easily solve this eigenvalue

Application



To find the eigenvalues of a complicated quantum graph, we can always "break it down" into trivial intervals, and iteratively we solve the eigenvalues.

Acknowledgement

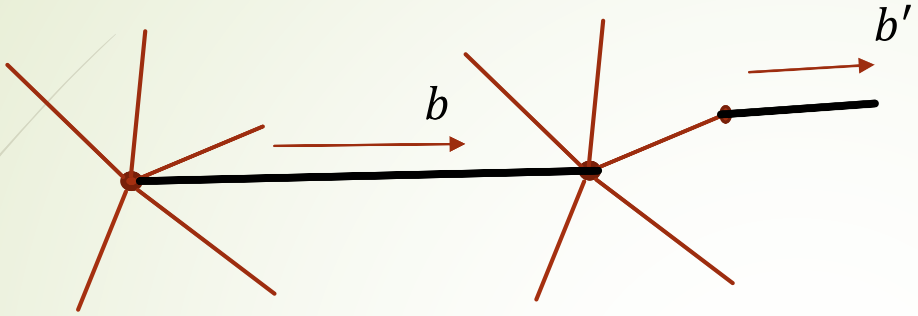
Supervisor: Professor Berkolaiko

An analogous result in the case of matrix

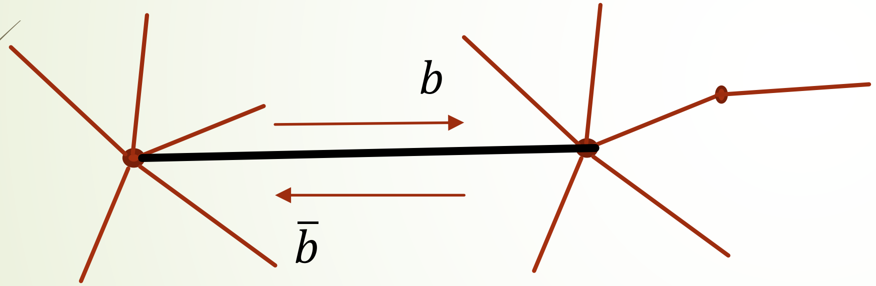
Theorem:

Define a vector $\vec{V} \in C^n$, obtained matrix B by $B = \vec{V} \cdot \vec{V}^T$, for any real Hermitian matrix $A \in C^{n \times n}$, we have the function $f(\lambda) = \frac{\det(A+B-\lambda I)}{\det(A-\lambda I)}$ has negative derivatives except for the locations λ is the eigenvalue for A.

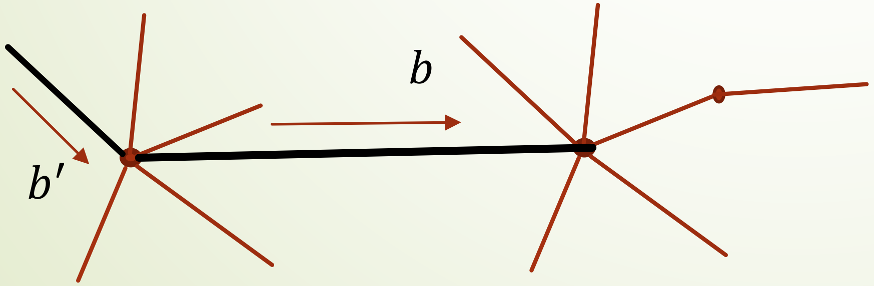
Secular Determinant



$$S_{b',b} = 0$$



$$S_{b',b} = \frac{2}{d} - 1 \quad \text{if } b' = \bar{b}$$



$$S_{b',b} = \frac{2}{d} \qquad \text{if } b' \text{ follows } b \text{ and } b' \neq \bar{b}$$