A Gelfand-Levitan Trace Formula for Generic Quantum Graphs

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joint work with P. Freitas

Graz, February 27, 2019

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[1] Support by the project "International mobilities for research activities of the University of Hradec Králové" CZ.02.2.69/0.0/0.0/16_027/0008487 and hospitality of the University of Lisbon during my stay is aknowledged.

Gelfand's and Levitan's result

- In 1953 Gelfand and Levitan[2] proved that for eigenvalues $\lambda_n(q)$ of the operator $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x)$ on $(0, \pi)$ with Neumann boundary conditions and eigenvalues $\lambda_n(0)$ of the same operator with $q = 0$ the following equality holds under the conditon $\int_0^\pi q(x)\,\mathrm{d}x = 0$

$$\sum_{n=1}^{\infty} [\lambda_n(q) - \lambda_n(0)] = \frac{1}{4}[q(\pi) + q(0)]\,.$$

[2] Gelfand, I. M. and Levitan, B., On a simple identity for the characteristic values of a differential operator of the second order. (Russian), *Doklady Akad. Nauk SSSR* **88** (1953), 593–596.

Generalization to q with non-zero average

- let us assume $\tilde{q}(x) = q(x) - \bar{q}$, where $\bar{q} = \frac{1}{\pi}\int_0^\pi q(x)\,\mathrm{d}x$
- the Schrödinger equation is

$$\begin{aligned} -u_n''(x) + q(x)u_n(x) &= \lambda_n(q)u_n(x)\,, \\ -u_n''(x) + \tilde{q}(x)u_n(x) &= (\lambda_n(q) - \bar{q})u_n(x) = \lambda_n(\tilde{q})u_n(x)\,. \end{aligned}$$

- moreover,

$$\frac{1}{4}[\tilde{q}(\pi)+\tilde{q}(0)] = \frac{1}{4}[q(\pi)-\bar{q}+q(0)-\bar{q}] = \frac{1}{4}[q(\pi)+q(0)]-\frac{1}{2}\bar{q}\,.$$

- we have

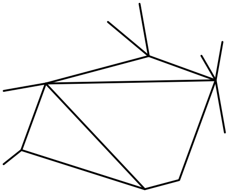
$$\sum_{n=1}^{\infty}\left[\lambda_n(q) - \lambda_n(0) - \frac{1}{\pi}\int_0^\pi q(x)\,\mathrm{d}x\right] = \frac{1}{4}[q(\pi)+q(0)]-\frac{1}{2\pi}\int_0^\pi q(x)\,\mathrm{d}x$$

Description of the model

- set of ordinary differential equations
- graph consists of set of vertices $\mathcal{V}$, set of d not oriented finite edges $\mathcal{E}$ (lengths of the edges are ℓ_j)
- Hilbert space of the problem

$$\mathcal{H} = \bigoplus_{j=1}^{d} L^2([0, \ell_j])$$

- the Hamiltonian acting as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q_j(x)$, where $q_j(x)$ is bounded – corresponds to the Hamiltonian of a quantum particle for the choice $\hbar = 1$, $m = 1/2$



Domain of the Hamiltonian

- domain consisting of functions in $W^{2,2}(\Gamma)$ satisfying coupling conditions at each vertex
- coupling conditions given by

$$(U_v - I_v)\Psi_v + i(U_v + I_v)\Psi'_v = 0\,.$$

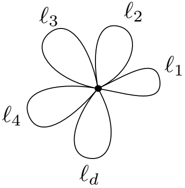
  where $\Psi_v = (\psi_1(0), \dots, \psi_{d_v}(0))^{\mathrm{T}}$ and $\Psi'_v = (\psi_1(0)', \dots, \psi_{d_v}(0)')^{\mathrm{T}}$ are the vectors of limits of functional values and outgoing derivatives where d_v is the number edges emanating from the vertex v and U_v is a unitary $d_v \times d_v$ matrix
- assume that $-1 \notin \sigma(U_v)$
- this set does not include Dirichlet, delta or standard coupling

Flower-like model

- description of coupling conditions using one-vertex graphs
- suppose that Γ has d edges of finite length
- the coupling condition

$$(U - I)\Psi + i(U + I)\Psi' = 0$$

  describes coupling on the whole graph; U is $2d \times 2d$ unitary matrix consisting of blocks U_v
- the above equation decouples into conditions for particular vertices
- U encodes not only coupling at the vertices, but also the topology of the graph



Generalizations of Gelfand's and Levitan's formula to graphs

- first attempts to obtain a trace formula for graphs by Roth [3]
- a formula involving integrals of the potential and the eigenfunctions by Carlson [4]
- results closer to Gelfand's and Levitan's formula: equilateral star graphs with different boundary conditions [5] [6], segment with discontinuity boundary conditions [7]

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[3] Roth, J.-P. Spectre du laplacien sur un graphe, *C.R. Acad. Sci. Paris* **296** (1983), 793795.

[4] Carlson, R. Eigenvalue cluster traces for quantum graphs with equal edge lengths Rocky Mountain. *J. Math.* **42** (2012), 467490.

[5] Yang, C.-F. Regularized trace for Sturm-Liouville differential operator on a star-shaped graph. Complex *Anal. Oper. Theory* **7** (2013), 11851196.

[6] Yang, C.-F. and Yang, J.-X. Large eigenvalues and traces of Sturm-Liouville equations on star-shaped graphs. *Methods Appl. Anal.* **14** (2007), 179196.

[7] Yang, C.-F. Traces of Sturm-Liouville operators with discontinuities. *Inverse Problems in Science and Engineering* **22** (2014), 803813.

Asymptotic behaviour of eigenvalues

- we subtract the eigenvalue for zero potential, not a known particular value – a more elegant result
- asymptotic behaviour of the spectrum: the leading term of the secular equation is $\prod_{i=1}^{d}(-k\sin(k\ell_i))$
- we obtain d sequences of eigenvalues in the following way: denote the sequence of all eigenvalues in increasing order by $\{\lambda_n\}_{n=1}^{\infty}$ and let the sequence $\{\mu_n\}_{n=1}^{\infty}$ correspond to the non-negative zeros of the above product also arranged in increasing order, with the first d entries being 0
- pair λ_n with μ_n
- define the subsequences $\{\lambda_{in}\}_{n=0}^{\infty}$ as subsequences of $\{\lambda_n\}_{n=1}^{\infty}$ which are paired with those zeros of $\prod_{i=1}^{d}(-k\sin(k\ell_i))$ which are positive zeros of $\sin(k\ell_i)$ for a given i (the first entry of this sequence λ_{i0} is paired with 0)

Main result

Theorem 1 (Freitas,L.)

We assume a quantum graph with d edges with arbitrary lengths ℓ_i, $i = 1, \ldots, d$, and associated coupling matrix U not having -1 in its spectrum. Then, denoting the eigenvalues of the Hamiltonian with a potential q and with the zero potential by $\lambda_{in}(q)$ and $\lambda_{in}(0)$, respectively, in the way described above, and the component of the potential on the i-th edge by $q_i \in W^{1,1}((0,\ell_i))$, the following trace formula holds

$$\sum_{i=1}^{d}\sum_{n=0}^{\infty}\left[\lambda_{in}(q) - \lambda_{in}(0) - \frac{1}{\ell_i}\int_0^{\ell_i} q_i(x)\,\mathrm{d}x\right] = \\ = \sum_{i=1}^{d}\left\{\frac{1}{4}\left[q_i(\ell_i) + q_i(0)\right] - \frac{1}{2\ell_i}\int_0^{\ell_i} q_i(x)\,\mathrm{d}x\right\}.$$

The secular equation

- we rewrite the coupling condition as

$$H\Psi + \Psi' = 0\,,$$

where $H = -i(U+I)^{-1}(U-I)$ is a Hermitian $2d \times 2d$ matrix

- independent solutions on the edges

$$c_j(x,k) = \cos(kx) + \int_0^x \frac{\sin(k(x-t))}{k} q_j(t) c_j(t,k)\,\mathrm{d}t\,,$$
$$s_j(x,k) = \frac{\sin(kx)}{k} + \int_0^x \frac{\sin(k(x-t))}{k} q_j(t) s_j(t,k)\,\mathrm{d}t\,.$$

- the solution on each edge can be expressed as

$$f_j(x) = A_j c_j(x,k) + B_j s_j(x,k)\,,$$

- we substitute this expression to the coupling conditions and obtain

$$[HM_1(k) + M_2(k)](A_1, B_1, A_2, B_2, \dots, A_d, B_d)^{\mathrm{T}} = 0\,.$$

$$M_1(k) = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ c_1(\ell_1,k) & s_1(\ell_1,k) & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & c_2(\ell_2,k) & s_2(\ell_2,k) & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$M_2(k) = \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ -c_1'(\ell_1,k) & -s_1'(\ell_1,k) & 0 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ 0 & 0 & -c_2'(\ell_2,k) & -s_2'(\ell_2,k) & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- the first three terms of the secular equation

$$0 = \varphi(k) = \prod_{i=1}^{d}(-k\sin(k\ell_i)) + \sum_{i=1}^{d}\left(\prod_{\substack{j=1\\ j\neq i}}^{d}(-k\sin(k\ell_j))\right)$$

$$[\cos(k\ell_i)(a_i - \mathrm{Tr}\,H_i) - 2\mathrm{Re}\,H_{12i}]+$$

$$+\sum_{\substack{i,j=1\\ i<j}}^{d}\left(\prod_{\substack{o=1\\ o\neq i,j}}^{d}(-k\sin(k\ell_o))\right)\left\{\frac{\sin(k\ell_i)\sin(k\ell_j)}{d-1}(a_i\mathrm{Tr}\,H_i + a_j\mathrm{Tr}\,H_j - \right.$$

$$-b_i - b_j - \det H_i - \det H_j) + \cos(k\ell_i)\cos(k\ell_j)[a_i a_j - a_i\mathrm{Tr}\,H_j -$$

$$-a_j\mathrm{Tr}\,H_i - (|H_{11ij}|^2 + |H_{12ij}|^2 + |H_{21ij}|^2 + |H_{22ij}|^2) + \mathrm{Tr}\,H_i\mathrm{Tr}\,H_j]+$$

$$+\cos(k\ell_i)[2(\mathrm{Tr}\,H_i - a_i)\mathrm{Re}\,H_{12j} - 2\mathrm{Re}\,(H_{11ij}\bar{H}_{12ij} + H_{22ij}\bar{H}_{21ij})]+$$

$$+\cos(k\ell_j)[2(\mathrm{Tr}\,H_j - a_j)\mathrm{Re}\,H_{12i} - 2\mathrm{Re}\,(H_{11ij}\bar{H}_{21ij} + H_{22ij}\bar{H}_{12ij})]+$$

$$\left. +4\mathrm{Re}\,H_{12i}\mathrm{Re}\,H_{12j} - 2\mathrm{Re}\,(H_{12ij}\bar{H}_{21ij} + H_{11ij}\bar{H}_{22ij})\right\} +$$

$$+\,\mathrm{o}\left(k^{d-2}\mathrm{e}^{|\mathrm{Im\,k}|\sum_{i=1}^{d}\ell_i}\right)\,.$$

Proof of the main result

Theorem 2 (Freitas,L.)

For all $\varepsilon > 0$ there exists $K > 0$ so that for all $N > K$ and $N \notin \cup_{i=1}^{d} \cup_{n\in\mathbb{N}_0} \left(\frac{n\pi}{\ell_i} - \frac{\varepsilon}{\ell_i}, \frac{n\pi}{\ell_i} + \frac{\varepsilon}{\ell_i}\right)$ the functions $\prod_{i=1}^{d}(-k\sin(k\ell_i))$ and $\varphi(k)$have the same number of zeros inside the contour Γ_N (counter-clockwise contour with vertices $N - iN$, $N + iN$, $-N + iN$, $-N - iN$).

- proof using the symmetric Rouché's theorem

Theorem 3 (Rouché)

Let f and g be holomorphic functions in the bounded subset V of $\mathbb{C}$ and continuous at its closure $\bar{V}$. Let us assume that on the boundary ∂V of V the following relation holds $|f - g| < |f| + |g|$. Then functions f and g have the same number of zeros in V.

Lemma 4 (Freitas,L.)

It is possible to choose $\varepsilon > 0$ and $K > 0$ such that there exists a strictly increasing sequence $\{N_p\}_{p=1}^{\infty}$ with $K < N_1$ and satisfying

$$N_p \notin \cup_{i=1}^{d} \cup_{n\in\mathbb{N}_0} \left(\frac{n\pi}{\ell_i} - \frac{\varepsilon}{\ell_i}, \frac{n\pi}{\ell_i} + \frac{\varepsilon}{\ell_i}\right)$$

and

$$\lim_{p\to\infty} N_p = +\infty.$$

and there are at most d eigenvalues $\lambda = k^2$ of $\mathcal{H}$ with $N_p \le k \le N_{p+1}$, for all $p \in \mathbb{N}$. Furthermore, all these eigenvalues belong to different sequences λ_{in} and there are at most d zeros μ of $\prod_{i=1}^{d} \sin(k\ell_i)$ with $N_p \le \mu \le N_{p+1}$, $\forall p \in \mathbb{N}$. The number of eigenvalues and zeros with this property is the same.

- C_p the counter-clockwise rectangles with vertices $N_{p+1} - iN_{p+1}$, $N_{p+1} + iN_{p+1}$, $N_p + iN_{p+1}$ and $N_p - iN_{p+1}$

Theorem 5 (Freitas,L.)

Let us assume that inside the contour C_p there are the points $\frac{n\pi}{\ell_i}$ and $k_{in} = \sqrt{\lambda_{in}}$ for a given i. Then $\lambda_{in} = k_{in}^2$ behaves asymptotically as

$$\lambda_{in} = \left(\frac{n\pi}{\ell_i}\right)^2 + \frac{2}{\ell_i}[a_i - \mathrm{Tr}\, H_i - (-1)^n 2\mathrm{Re}\, H_{12i}] +$$

$$+ \frac{2}{n\pi} \sum_{\substack{j=1 \\ j\neq i}}^{d} \Bigg[\cot \frac{n\pi\ell_j}{\ell_i}(|H_{11ij}|^2 + |H_{12ij}|^2 + |H_{21ij}|^2 + |H_{22ij}|^2) +$$

$$+ \frac{1}{\sin \frac{n\pi\ell_j}{\ell_i}} 2\mathrm{Re}\,(H_{11ij}\bar{H}_{12ij} + H_{22ij}\bar{H}_{21ij}) +$$

$$\frac{(-1)^n}{\sin \frac{n\pi\ell_j}{\ell_i}} 2\mathrm{Re}\,(H_{12ij}\bar{H}_{21ij} + H_{11ij}\bar{H}_{22ij}) +$$

$$(-1)^n \cot \frac{n\pi\ell_j}{\ell_i} 2\mathrm{Re}\,(H_{11ij}\bar{H}_{21ij} + H_{22ij}\bar{H}_{12ij})\Bigg] + \mathrm{O}\left(\frac{1}{n^2}\right).$$

Corollary 6 (Freitas,L.)

The sum

$$\sum_{i=1}^{d} \sum_{n=0}^{\infty} \left[\lambda_{in}(q) - \lambda_{in}(0) - \frac{2a_i}{\ell_i} \right]$$

is absolutely convergent, where $\lambda_{in}(q)$ *and and* $\lambda_{in}(0)$ *denote the eigenvalues for the potential* q *and for the null potential, respectively.*

- idea of the proof: subtracting *rhs* of the equation in Theorem 5
- the term with $1/n$ depends only on H, not on the potential

Proof of Theorem 1

- we choose the contours Γ_N in the "allowed regions" with $N \to \infty$
- for sufficiently large N, there are $d + \sum_{i=1}^{d} \left\lfloor \frac{N\ell_i}{\pi} \right\rfloor$ eigenvalues
- the number of k_n with $k_n^2 = \lambda_n$ is double
- we have

$$2 \sum_{i=1}^{d} \sum_{n=0}^{\lfloor \frac{N\ell_i}{\pi} \rfloor} [\lambda_{in}(q) - \lambda_{in}(0)] = -\frac{1}{2\pi i} \oint_{\Gamma_N} \ln \frac{\varphi(k)}{\varphi_0(k)} 2k \, \mathrm{d}k \, .$$

- we send N to infinity

Paper on which the talk was based

P. Freitas, J. Lipovský: A Gelfand-Levitan trace formula for generic quantum graphs, arXiv: 1901.07790 [math-ph]

Thank you for your attention!

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