On the effective size of a non-Weyl graph

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Ostrava, 22nd March 2016

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[1] Support of project 15-14180Y "Spectral and resonance properties of quantum models" of the Grant Agency of the Czech Republic is acknowledged.

Outline

- Introduction
- Previous results on resonance asymptotics on quantum graphs
- Pseudo orbit expansion
- Example: triangle with attached halflines
- Deleting edges of the directed graph
- Example revisited: triangle with attached halflines
- Main results on the effective size

Description of the model

- set of ordinary differential equations
- graph consists of set of vertices $\mathcal{V}$, set of not oriented edges (both finite $\mathcal{E}$ and infinite $\mathcal{E}_\infty$).
- Hilbert space of the problem

$$\mathcal{H} = \bigoplus_{(j,n)\in I_{\mathcal{L}}} L^2([0,l_{jn}]) \oplus \bigoplus_{j\in I_{\mathcal{C}}} L^2([0,\infty))\,.$$

- states described by columns

$$\psi = (f_{jn} : \mathcal{E}_{jn} \in \mathcal{E},\; f_{j\infty} : \mathcal{E}_{j\infty} \in \mathcal{E}_\infty)^T .$$

- the Hamiltonian acting as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$, where $V(x)$ is bounded and supported only on the internal edges – 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 $\Psi_v = (\psi_1(0), \dots, \psi_d(0))^{\mathrm{T}}$ and $\Psi'_v = (\psi_1(0)', \dots, \psi_d(0)')^{\mathrm{T}}$ are the vectors of limits of functional values and outgoing derivatives where d is the number edges emanating from the vertex v and U_v is a unitary $d \times d$ matrix

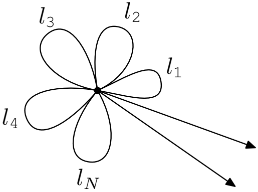
- in particular, standard (Kirchhoff) coupling conditions: $f_i(v) = f_j(v)$, $\sum_{j=1}^{d} f'_j(v) = 0$.

Flower-like model

- description of coupling conditions using one-vertex graphs
- suppose that Γ has N internal and M external edges
- the coupling condition

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

  describes coupling on the whole graph; U is $(2N+M)\times(2N+M)$ 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



Effective coupling on a finite graph

- replacing non-compact graph by its compact part
- instead of halflines there are effective coupling matrices
- N internal, M external edges – U consists of blocks U_j

$$U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix} ,$$

  where U_1 is $2N \times 2N$ matrix corresponding to coupling between internal edges, etc.

- by a standard procedure (Schur, etc.) one gets an effective coupling matrix

$$\tilde{U}(k) = U_1 - (1-k)U_2[(1-k)U_4 - (k+1)I]^{-1}U_3$$

- coupling condition has the same form only with U replaced by $\tilde{U}(k)$

$$(\tilde{U}(k) - I)\Psi_1 + i(\tilde{U}(k) + I)\Psi_1' = 0$$

Resolvent resonances

- poles of the meromorphic continuation of the resolvent $(H - \lambda \mathrm{id})^{-1}$
- can be obtained by the external complex scaling – transformation external components of the wavefunction

$$g_j(x) \mapsto U_\theta g_j(x) = \mathrm{e}^{\theta/2} g_j(x\mathrm{e}^\theta)$$

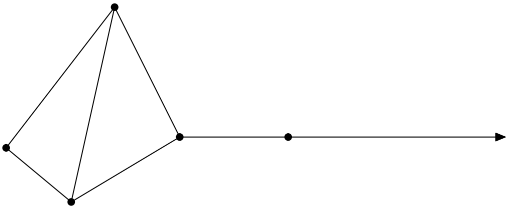
  with a nontrivial imaginary part of θ
- another definition: $\lambda = k^2$ is a resolvent resonance if there exists a generalized eigenfunction $f \in L^2_{\mathrm{loc}}(\Gamma)$, $f \not\equiv 0$ satisfying $-f''(x) = k^2 f(x)$ on all edges of the graph and fulfilling the coupling conditions, which on all external edges behaves as $c_j\, \mathrm{e}^{ikx}$.

Asymptotics of resonances on quantum graphs

- $N(R)$ number of resolvent resonances in the circle of radius R in the k plane
- expected behaviour of the counting function

$$N(R) = \frac{2\mathrm{vol}\,(\Gamma)}{\pi} R + \mathcal{O}(1)$$

- trivial example of a graph where this asymptotics is not satisfied



Asymptotics for standard conditions

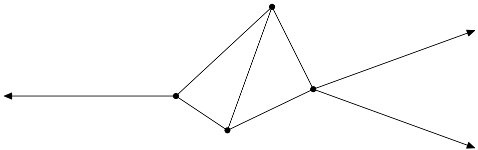
Theorem (Davies, Pushnitski)

Suppose that Γ is the graph with standard (Kirchhoff) coupling conditions at all the vertices. Then

$$N(R) = \frac{2}{\pi} W R + O(1)\,, \quad \text{as } R \to \infty,$$

where the coefficient W satisfies $0 \le W \le \mathrm{vol}\,(\Gamma)$. The behaviour is non-Weyl ($0 \le W < \mathrm{vol}\,(\Gamma)$) iff there is a balanced vertex.

- $\mathrm{vol}\,(\Gamma)$ is sum of lengths of the internal edges
- balanced vertex: number of internal edges is equal to the number of external edges



Zeros of exponential polynomials

Theorem (Langer)

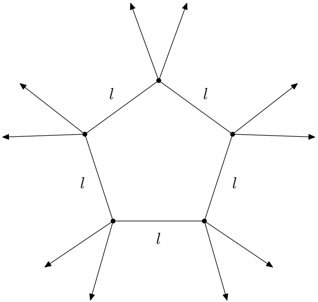
Let us assume an exponential polynomial $F(k) = \sum_{r=0}^{n} k^{\nu_r} a_r(k) \mathrm{e}^{ik\sigma_r}$*, where* $\nu_r \in \mathbb{R}$*,* $a_r(k)$ *are rational functions of the complex variable* k *with complex coefficients which do not vanish identically and* $\sigma_r \in \mathbb{R}$*,* $\sigma_0 < \sigma_1 < \cdots < \sigma_n$*. Suppose that* $\lim_{k\to\infty} a_r(k) = \alpha_r$ *are finite and nonzero for all* r*. Then the counting function of the number of zeros of the function* $F(k)$ *in the circle of radius* R *behaves as*

$$N(R, F) = \frac{\sigma_n - \sigma_0}{\pi} R + \mathcal{O}(1)$$

for $R \to \infty$*.*

Effective size of a graph – example

- regular polygon with two halflines attached at each vertex



- criterion whether the graph is Weyl or non-Weyl is local, while the effective size of a non-Weyl graph depends on topology of the whole graph

- using the unitary rotation operator and the Bloch-Floquet decomposition with respect to the cyclic rotational group one can find the final resonance condition for each element of the graph

$$-2(\omega^2+1)+4\omega \mathrm{e}^{-ik\ell}=0.$$

  with ω satisfying $\omega^n = 1$
- hence the middle term is zero iff $\omega = \pm i$

$$W_n = \begin{cases} n\ell/2 & \text{if } n \neq 0 \mod 4, \\ (n-2)\ell/2 & \text{if } n = 0 \mod 4. \end{cases}$$

Pseudo orbit expansion for the resonance condition

- there is a known method for finding the spectrum of a compact graph by the pseudo orbit expansion
- the vertex scattering matrix maps the vector of amplitudes of the incoming waves into a vector of amplitudes of the outgoing waves $\vec{\alpha}_v^{\mathrm{out}} = \sigma^{(v)} \vec{\alpha}_v^{\mathrm{in}}$
- for a non-compact graph we similarly define effective vertex scattering matrix $\tilde{\sigma}^{(v)}$

Theorem

Let us assume the vertex connecting n internal and m external edges. The effective vertex-scattering matrix is given by

$$\tilde{\sigma}(k) = -[(1-k)\tilde{U}(k) - (1+k)I_n]^{-1}[(1+k)\tilde{U}(k) - (1-k)I_n]$$

In particular, for the standard conditions we have $\tilde{\sigma}(k) = \frac{2}{n+m} J_n - I_n$*, where* J_n *denotes* $n \times n$ *matrix with all entries equal to one. For a balanced vertex we have* $\tilde{\sigma}(k) = \frac{1}{n} J_n - I_n$.

- idea of the pseudo orbit expansion: replacing the compact part of the graph Γ by a oriented graph Γ_2, each edge replaced by two bonds b, $\hat{b}$
- ansatz

$$f_{b_j}(x) = \alpha_{b_j}^{\mathrm{in}} \mathrm{e}^{-ikx} + \alpha_{b_j}^{\mathrm{out}} \mathrm{e}^{ikx}\,,$$
$$f_{\hat{b}_j}(x) = \alpha_{\hat{b}_j}^{\mathrm{in}} \mathrm{e}^{-ikx} + \alpha_{\hat{b}_j}^{\mathrm{out}} \mathrm{e}^{ikx}$$

- due to the relation $f_{b_j}(x) = f_{\hat{b}_j}(\ell_j - x)$ we have

$$\alpha_{b_j}^{\mathrm{in}} = \mathrm{e}^{ik\ell_j} \alpha_{\hat{b}_j}^{\mathrm{out}}\,, \qquad \alpha_{\hat{b}_j}^{\mathrm{in}} = \mathrm{e}^{ik\ell_j} \alpha_{b_j}^{\mathrm{out}}\,.$$

- we define $\tilde{\Sigma}(k)$ as a block-diagonalizable matrix written in the basis corresponding to

$$\vec{\alpha} = (\alpha_{b_1}, \dots, \alpha_{b_N}, \alpha_{\hat{b}_1}, \dots, \alpha_{\hat{b}_N})^{\mathrm{T}}$$

which is block diagonal with blocks $\tilde{\sigma}_v(k)$ if transformed to the basis

$$(\alpha_{b_{v_1 1}}^{\mathrm{in}}, \dots, \alpha_{b_{v_1 d_1}}^{\mathrm{in}}, \alpha_{b_{v_2 1}}^{\mathrm{in}}, \dots, \alpha_{b_{v_2 d_2}}^{\mathrm{in}}, \dots,)^{\mathrm{T}}.$$

- we define

$$Q = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},$$

scattering matrix $S = Q\tilde{\Sigma}$ and

$$L = \mathrm{diag}\,(\ell_1, \dots, \ell_N, \ell_1, \dots, \ell_N)$$

- we obtain

$$\begin{pmatrix} \vec{\alpha}_b^{\mathrm{in}} \\ \vec{\alpha}_{\hat{b}}^{\mathrm{in}} \end{pmatrix} = \mathrm{e}^{ikL} \begin{pmatrix} \vec{\alpha}_{\hat{b}}^{\mathrm{out}} \\ \vec{\alpha}_b^{\mathrm{out}} \end{pmatrix} = \mathrm{e}^{ikL} Q \begin{pmatrix} \vec{\alpha}_b^{\mathrm{out}} \\ \vec{\alpha}_{\hat{b}}^{\mathrm{out}} \end{pmatrix} = \mathrm{e}^{ikL} Q\tilde{\Sigma}(k) \begin{pmatrix} \vec{\alpha}_b^{\mathrm{in}} \\ \vec{\alpha}_{\hat{b}}^{\mathrm{in}} \end{pmatrix}$$

- the resonance condition therefore is

$$\det\,(\mathrm{e}^{ikL} Q\tilde{\Sigma}(k) - I_{2N}) = 0$$

- **periodic orbit** γ is a closed path on Γ_2
- **pseudo orbit** $\tilde{\gamma}$ is a collection of periodic orbits
- **irreducible pseudo orbit** $\bar{\gamma}$ is a pseudo orbit, which does not use any directed edge more than once
- we define length of a periodic orbit by $\ell_\gamma = \sum_{j, b_j \in \gamma} \ell_j$; the length of pseudo orbit (and hence irreducible pseudo orbit) is the sum of the lengths of the periodic orbits from which it is composed
- we define product of scattering amplitudes for a periodic orbit $\gamma = (b_1, b_2, \dots, b_n)$ as $A_\gamma = S_{b_2 b_1} S_{b_3 b_2} \dots S_{b_1 b_n}$, where $S_{b_2 b_1}$ is the entry of the matrix S in the b_2-th row and b_1-th column; for a pseudo orbit we define $A_{\tilde{\gamma}} = \Pi_{\gamma_n \in \tilde{\gamma}} A_{\gamma_j}$
- by $m_{\tilde{\gamma}}$ we denote the number of periodic orbits in the pseudo orbit $\tilde{\gamma}$

- reformulation of the theorem on the resonance condition

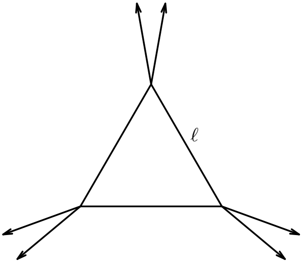
Theorem

The resonance condition is given by the sum over irreducible pseudo orbits

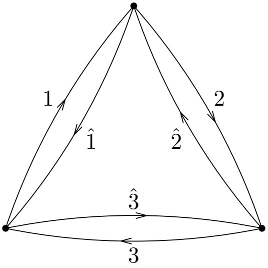
$$\sum_{\bar\gamma}(-1)^{m_{\bar\gamma}} A_{\bar\gamma}\, \mathrm{e}^{ik\ell_{\bar\gamma}} = 0\,.$$

- in general $A_{\bar\gamma}$ can be energy dependent, but this is not the case for standard coupling.
- idea of the proof: the permutations in the determinant can be represented as product of disjoint cycles

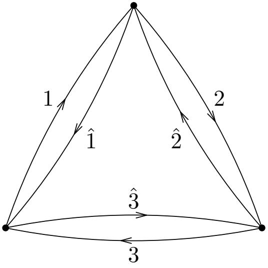
Example: triangle with attached halflines



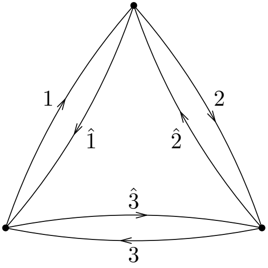
- the same lengths of the internal edges ℓ, standard coupling at all vertices
- the vertex scattering matrix is $\tilde{\sigma}^{(v)} = \frac{1}{2}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$



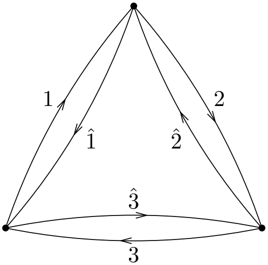
- the irreducible pseudo orbit on 0 edges
- contribution: 1



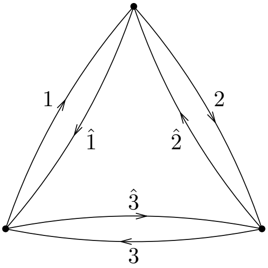
- the irreducible pseudo orbits on 2 edges: $(1\hat{1})$; $(2\hat{2})$; $(3\hat{3})$
- contribution: the coefficient by $\exp(2ik\ell)$ is $\left(-\frac{1}{2}\right)^2(-1)^1 \cdot 3 = -\frac{3}{4}$



- the irreducible pseudo orbits on 3 edges: $(1, 2, 3)$ and $(\hat{1}, \hat{3}, \hat{2})$
- contribution: the coefficient by $\exp(3ik\ell)$ is $\left(\frac{1}{2}\right)^3 (-1)^1 \cdot 2 = -\frac{1}{4}$

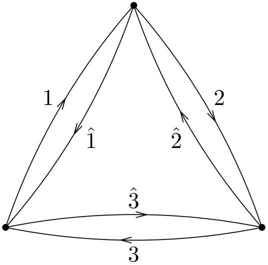


- the irreducible pseudo orbits on 4 edges: $(1,\hat{1})(2,\hat{2})$; $(1,\hat{1})(3,\hat{3})$; $(3,\hat{3})(2,\hat{2})$; $(1,2,\hat{2},\hat{1})$; $(2,3,\hat{3},\hat{2})$ and $(3,1,\hat{1},\hat{3})$
- contribution: the coefficient by $\exp(4ik\ell)$ is $\left(-\frac{1}{2}\right)^4(-1)^2\cdot 3+\left(-\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^2(-1)^1\cdot 3=0$



- the irreducible pseudo orbits on 6 edges: $(1,\hat{1})(2,\hat{2})(3,\hat{3})$; $(1,2,\hat{2},\hat{1})(3,\hat{3})$; $(2,3,\hat{3},\hat{2})(1,\hat{1})$; $(3,1,\hat{1},\hat{3})(2,\hat{2})$; $(1,2,3)(\hat{1},\hat{3},\hat{2})$; $(1,2,3,\hat{3},\hat{2},\hat{1})$; $(2,3,1,\hat{1},\hat{3},\hat{2})$; $(3,1,2,\hat{2},\hat{1},\hat{3})$
- contribution: the coefficient by $\exp(6ik\ell)$

$$\left(-\frac{1}{2}\right)^6(-1)^3+\left(-\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^2\left(-\frac{1}{2}\right)^2(-1)^2\cdot 3+$$
$$+\left(\frac{1}{2}\right)^3\left(\frac{1}{2}\right)^3(-1)^2+\left(-\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^4(-1)^1\cdot 3=0$$



- the resonance condition is

$$1 - \frac{3}{4}\exp\left(2ik\ell\right) - \frac{1}{4}\exp\left(3ik\ell\right) = 0\,.$$

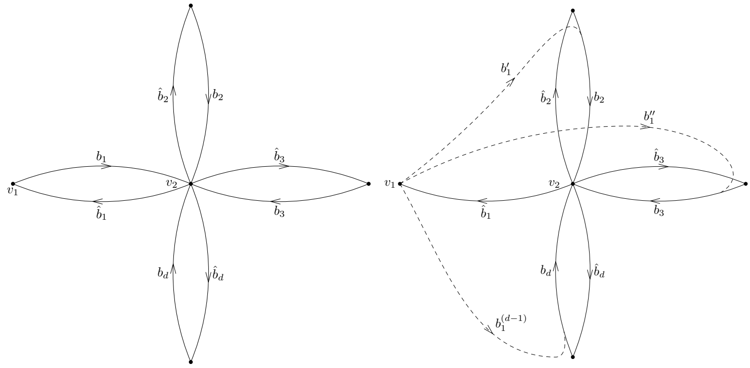
- the effective size is $3\ell/2$

Deleting edges of the graph and "ghost edges"

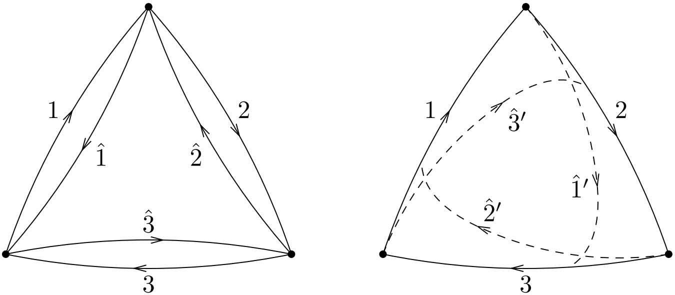
- method how to simplify the graph Γ_2 and find the resonance condition more easily for a non-Weyl graph
- assumptions: equilateral graph Γ for which no edge starts and ends in one vertex and no two vertices are connected by more than one edge
- standard coupling
- let there be a balanced vertex v_2 in which directed edges $b_1, b_2, \ldots, b_d$ end

Theorem

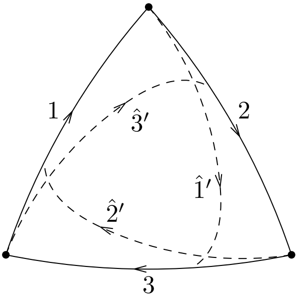
The following construction does not change the resonance condition. We delete the directed edge b_1 of the graph Γ_2, which starts in the vertex v_1, and replace it by "ghost edges" $b_1', b_1'', \dots, b_1^{(d-1)}$, where the "ghost edge" $b_1^{(j)}$ starts in the vertex v_1 and continues to the directed edge b_{j+1}. Contribution of the irreducible pseudo orbit containing "ghost edge" b_1' to the resonance condition is following. The ghost edge does not contribute to the length of the pseudo orbit. The scattering amplitude from the bond b, which ends in v_1, to the bond b_2 is equal to the scattering amplitude from b to b_1 taken with the opposite sign. Every "ghost edge" can be in the irreducible pseudo orbit used only once. Similarly, one can delete more edges; for each balanced vertex we delete an edge which ends in this vertex.


v_1
v_2
b_1
$\hat{b}_1$
b_2
$\hat{b}_2$
b_3
$\hat{b}_3$
b_d
$\hat{b}_d$
b_1'
b_1''
$b_1^{(d-1)}$

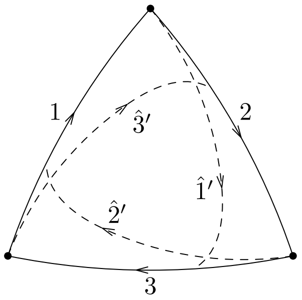
Example revisited



- we have deleted three edges; there are three new "ghost edges"
- pseudo orbit expansion for the graph with deleted edges
- irreducible pseudo orbits on zero edges: the contribution is 1



- irreducible pseudo orbits on two "non-ghost" edges: $(1, 2, \hat{2}')$; $(2, 3, \hat{3}')$; $(3, 1, \hat{1}')$
- contribution: the coefficient by $\exp(2ik\ell)$ is $\left(\frac{1}{2}\right)^2 (-1)^1 \cdot 3 = -\frac{3}{4}$



- irreducible pseudo orbits on three "non-ghost" edges: $(1, 2, 3)$ and $(1, \hat{1}', 3, \hat{3}', 2, \hat{2}')$
- contribution: the coefficient by $\exp(3ik\ell)$ is $\left(\frac{1}{2}\right)^3 (-1)^1 \cdot 2 = -\frac{1}{4}$
- there are no irreducible pseudo orbits on more edges
- the resonance condition is same as previously

Criterion for a non-Weyl graph

Theorem

The graph is non-Weyl iff $\det \tilde{\Sigma}(k) = 0$ *for all* $k \in \mathbb{C}$. *In other words, the graph is non-Weyl iff there exists a vertex for which* $\det \tilde{\sigma}_v(k) = 0$ *for all* $k \in \mathbb{C}$.

- we start with the resonance condition $\det\left(\mathrm{e}^{ikL} Q \tilde{\Sigma}(k) - I_{2N}\right) = 0$
- the leading term is $\det\left[Q\tilde{\Sigma}(k)\right] \mathrm{e}^{2ik\sum_{j=1}^{N} \ell_j}$, the term with the lowest multiple of ik is 1.
- alternative proof of theorem of Davies and Pushnitski
- for standard conditions $\tilde{\sigma}_v(k) = \frac{1}{n} J - I$

Effective size for the equilateral graph

Theorem

Let Γ be an equilateral graph (with all internal edges of length ℓ). Then the effective size of this graph is $\frac{\ell}{2} n_{\mathrm{nonzero}}$, where n_{nonzero} is the number of nonzero eigenvalues of the matrix $Q\tilde{\Sigma}$. Note that the rank of the matrix cannot be used instead of number of nonzero eigenvalues, because the matrix often has a Jordan form.

idea of the proof

- if there is n_{zero} eigenvalues of $Q\tilde{\Sigma}$, then one has to take n_{zero} entries from the unit matrix to the determinant

Main results

Theorem

Let us assume the equilateral graph (lengths ℓ) with standard coupling. Then its effective size is $W \leq N\ell - \frac{\ell}{2} n_{\mathrm{bal}} - \frac{\ell}{2} n_{\mathrm{nonneigh}}$, where n_{bal} is the number of balanced vertices and n_{nonneigh} is the number of balanced vertices which do not neighbour any other balanced vertex.

- for each balanced vertex one directed edge entering this vertex can be deleted
- in the balanced vertex of the degree d which do not neighbour any other balanced vertex we have $d - 1$ incoming directed bonds and d outgoing directed bonds
- no ghost edge ends in the outgoing edge
- for each balanced vertex one directed edge cannot be used in the irreducible pseudo orbit

Theorem

Let us assume the equilateral graph (lengths ℓ) with standard coupling which contains four balanced vertices which form a square (vertex 1 is connected with 2, 2 with 3, 3 with 4, 4 with 1, but vertex 1 is not connected with 3 and 2 is not connected with 4). Then the effective size is $W \leq (N-3)\ell$.

- we delete four directed edges of the square
- we use the symmetry of the graph with "ghost edges" and cancellation of contributions of some irreducible pseudo orbits

Theorem

Let us assume an equilateral graph (lengths ℓ) with standard coupling. Let the eigenvalues of $Q\tilde{\Sigma}$ be $c_j = r_j \mathrm{e}^{i\varphi_j}$. Then the resolvent resonances are $\lambda = k^2$ with $k = \frac{1}{\ell}(-\varphi_j + 2n\pi + i \ln r_j)$, $n \in \mathbb{Z}$. Moreover, $|c_j| \leq 1$ and for a graph with no edge starting and ending in one vertex also $\sum_{j=1}^{2N} c_j = 0$.

- the resonance condition is

$$\prod_{j=1}^{2N} (\mathrm{e}^{ik\ell} c_j - 1) = 0\,,$$

- hence we have

$$r_j \mathrm{e}^{-k_{\mathrm{I}}\ell} \mathrm{e}^{ik_{\mathrm{R}}\ell} \mathrm{e}^{i\varphi_j} = 1\,,$$

- if the graph does not have any edge starting and ending in one vertex, then there are zeros on the diagonal of $Q\tilde{\Sigma}$

Thank you for your attention!

Articles on which the talk was based

E.B. Davies, A. Pushnitski: Non-Weyl Resonance Asymptotics for Quantum Graphs, *Analysis and PDE* **4** (2011), no. 5, pp. 729-756. arXiv:1003.0051.

E.B. Davies, P. Exner, J. Lipovský: Non-Weyl asymptotics for quantum graphs with general coupling conditions *J. Phys. A* **43** (2010), 474013. arXiv: 1004.0856.

J. Lipovský: On the effective size of a non-Weyl graph, arXiv: 1507.04176 [math-ph].

J. Lipovský: Pseudo orbit expansion for the resonance condition on quantum graphs and the resonance asymptotics *Acta Physica Polonica A* **128** (2015), no. 6, p. 968 973. arXiv: 1507.06845

R. Band, J. M. Harrison, and C. H. Joyner: Finite pseudo orbit expansion for spectral quantities of quantum graphs. *J. Phys. A: Math. Theor.* **45** (2012), p. 325204