Resonances in quantum networks

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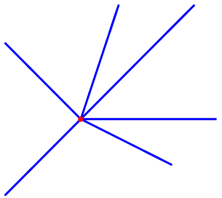
- How *magnetic field* can influence high-energy resonance asymptotics
- *Generalized quantum graphs*: equivalence of resonance definitions and *magnetic field influence* again

The coupling in quantum graph vertices



The most simple example is a *star graph* with the state Hilbert space $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and the particle Hamiltonian acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j''$

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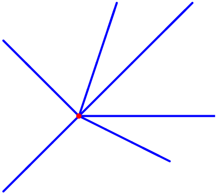

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Since it is second-order, the boundary condition involve $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$ being of the form

$$A\Psi(0) + B\Psi'(0) = 0\,;$$

by [Kostrykin-Schrader'99] the $n \times n$ matrices A, B give rise to a self-adjoint operator if they satisfy the conditions

- $\mathrm{rank}\,(A, B) = n$
- AB^* is self-adjoint

Unique form of boundary conditions

The non-uniqueness of the above b.c. can be removed:

Proposition (Harmer'00, K-S'00)

Vertex couplings are uniquely characterized by unitary $n \times n$ matrices U such that

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Self-adjointness requires vanishing of the boundary form,

$$\sum_{j=1}^{n} (\bar\psi_j \psi_j' - \bar\psi_j' \psi_j)(0) = 0\,,$$

which occurs *iff* the norms $\|\Psi(0) \pm i\ell\Psi'(0)\|_{\mathbb{C}^n}$ with a fixed $\ell \neq 0$ coincide, so the vectors must be related by an $n \times n$ unitary matrix; this gives $(U - I)\Psi(0) + i\ell(U + I)\Psi'(0) = 0$.

Examples of vertex coupling

- Denote by $\mathcal{J}$ the $n \times n$ matrix whose all entries are equal to one; then $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ corresponds to the standard *δ coupling*,

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,,\; j,k = 1,\dots,n\,,\;\; \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0)$$

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- $\alpha = 0$ corresponds to the "free motion", the so-called *free boundary conditions* (better name than Kirchhoff)
- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *δ_s' coupling*

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with $\beta \in \mathbb{R}$; for $\beta = \infty$ we get *Neumann* decoupling

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- and *a lot* more

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- Most typical resonance situations arise for *finite graphs with semiinfinite leads*
- *Different resonances definitions:* poles of continued resolvent, singularities of on-shell S matrix
- Graphs may exhibit embedded eigenvalues due to *invalidity of uniform continuation*
- Frequent appearance of resonances and relative easiness to treat them make quantum graphs *natural laboratory* to study these effects

Preliminaries

Consider a graph Γ consisting of families od vertices $\mathcal{V} = \{\mathcal{X}_j : j \in I\}$, finite edges $\mathcal{L} = \{\mathcal{L}_{jn} : (\mathcal{X}_j, \mathcal{X}_n) \in I_{\mathcal{L}} \subset I \times I\}$, and infinite edges $\mathcal{L}_\infty = \{\mathcal{L}_{j\infty} : \mathcal{X}_j \in I_{\mathcal{C}}\}$. The corresponding state Hilbert space is

$$\mathcal{H} = \bigoplus_{L_j \in \mathcal{L}} L^2([0, l_j]) \oplus \bigoplus_{\mathcal{L}_{j\infty} \in \mathcal{L}_\infty} L^2([0, \infty))\,;$$

its elements are columns $\psi = (f_j : \mathcal{L}_j \in \mathcal{L},\, g_j : \mathcal{L}_{j\infty} \in \mathcal{L}_\infty)^T$.

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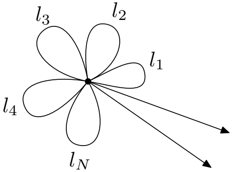
The Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$ on each link on $\mathcal{H}^2_{\mathrm{loc}}$ functions satisfying the boundary conditions

$$(U_j - I)\Psi_j + i(U_j + I)\Psi_j' = 0$$

characterized by unitary matrices U_j at the vertices $\mathcal{X}_j$.

A universal setting for graphs with leads

A useful trick is to replace Γ "flower-like" graph with one vertex by putting all the vertices to a single point,



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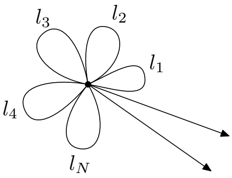

Its degree is $2N + M$ where $N := \mathrm{card}\,\mathcal{L}$ and $M := \mathrm{card}\,\mathcal{L}_\infty$

The coupling is described by "big", $(2N + M) \times (2N + M)$ unitary block diagonal matrix U consisting of blocks U_j as follows,

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

the block structure of U encodes the original topology of Γ.

Equivalence of different resonance definitions

Resonances as poles of analytically continued resolvent, $(H - \lambda\,\mathrm{id})^{-1}$. One way to reveal the poles is to use *exterior complex scaling*. Looking for complex eigenvalues of the scaled operator we do not change the compact part of the graph: we set $f_j(x) = a_j \sin kx + b_j \cos kx$ on the j-th internal edge

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On the other hand, functions on the semi-infinite edges are scaled by $g_{j\theta}(x) = \mathrm{e}^{\theta/2} g_j(x\mathrm{e}^{\theta})$ with an imaginary θ rotating the essential spectrum into the lower complex halfplane so that the poles of the resolvent on the second sheet become "uncovered" for θ large enough. The "exterior" boundary values at energy k^2 are thus equal to

$$g_j(0) = \mathrm{e}^{-\theta/2} g_{j\theta}, \quad g_j'(0) = ik\mathrm{e}^{-\theta/2} g_{j\theta}$$

Resolvent resonances

Substituting into the boundary conditions we get

$$(U-I)C_1(k)\begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ \mathrm{e}^{-\theta/2}g_{1\theta} \\ \vdots \\ \mathrm{e}^{-\theta/2}g_{M\theta} \end{pmatrix} + ik(U+I)C_2(k)\begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ \mathrm{e}^{-\theta/2}g_{1\theta} \\ \vdots \\ \mathrm{e}^{-\theta/2}g_{M\theta} \end{pmatrix} = 0,$$

where $C_j := \mathrm{diag}\,(C_j^{(1)}(k), C_j^{(2)}(k), \dots, C_j^{(N)}(k), i^{j-1}I_{M\times M})$, with

$$C_1^{(j)}(k) = \begin{pmatrix} 0 & 1 \\ \sin kl_j & \cos kl_j \end{pmatrix}, \qquad C_2^{(j)}(k) = \begin{pmatrix} 1 & 0 \\ -\cos kl_j & \sin kl_j \end{pmatrix}$$

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Complex k which solve this condition indicate the resonance positions

Scattering resonances

In this case we choose conventionally a combination of two planar waves, $g_j = c_j \mathrm{e}^{-ikx} + d_j \mathrm{e}^{ikx}$, as an Ansatz on the external edges; we ask about poles of the matrix $S = S(k)$ which maps the amplitudes of the incoming waves $c = \{c_n\}$ into amplitudes of the outgoing waves $d = \{d_n\}$ by the relation $d = Sc$.

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$$(U - I)C_1(k) \begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ c_1 + d_1 \\ \vdots \\ c_M + d_M \end{pmatrix} + ik(U + I)C_2(k) \begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ d_1 - c_1 \\ \vdots \\ d_M - c_M \end{pmatrix} = 0$$

Equivalence of both resonance definitions

Since we are interested in zeros of $\det S^{-1}$, we regard the above relation as an equation for variables a_j, b_j and d_j while c_j are just parameters. Eliminating the variables a_j, b_j one derives from here a system of M equations expressing the map $S^{-1}d = c$. It is *not* solvable, $\det S^{-1} = 0$, provided

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This is the same condition as for the previous system of equations, hence we are able to conclude:

Proposition (E-Lipovský'10)

The two above resonance notions, the resolvent and scattering one, are equivalent for quantum graphs.

Effective coupling on compact part of the graph

The problem can be reduced to the compact subgraph only. We write U in the block form, $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$, where U_1 is the $2N \times 2N$ refers to the compact subgraph, U_4 is the $M \times M$ matrix related to the exterior part, and U_2 and U_3 are rectangular matrices connecting the two.

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Eliminating the external part leads to an effective coupling on the compact subgraph expressed by the condition

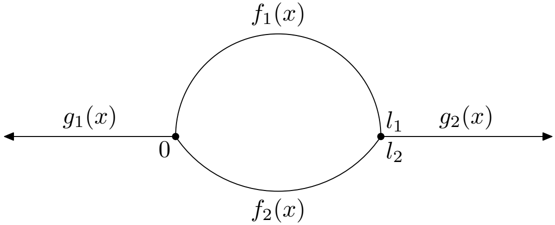
$$(\tilde{U}(k) - I)(f_1, \dots, f_{2N})^{\mathrm{T}} + i(\tilde{U}(k) + I)(f_1', \dots, f_{2N}')^{\mathrm{T}} = 0\,,$$

where the corresponding coupling matrix

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

is obviously *energy-dependent* and, in general, *non-unitary*

A geometric perturbation: a loop with two leads



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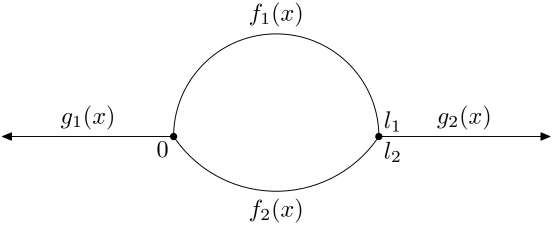

The setting is as above, the boundary condition at the nodes are

$$
\begin{aligned}
f_1(0) = f_2(0)\,, \qquad f_1(l_1) &= f_2(l_2)\,, \\
f_1(0) &= \alpha_1^{-1}(f_1'(0) + f_2'(0)) + \gamma_1 g_1'(0)\,, \\
f_1(l_1) &= -\alpha_2^{-1}(f_1'(l_1) + f_2'(l_2)) + \gamma_2 g_2'(0)\,, \\
g_1(0) &= \bar\gamma_1(f_1'(0) + f_2'(0)) + \tilde\alpha_1^{-1} g_1'(0)\,, \\
g_2(0) &- -\bar\gamma_2(f_1'(l_1) + f_2'(l_2)) + \tilde\alpha_2^{-1} g_2'(0)\,.
\end{aligned}
$$

Resonance condition

Writing the loop edges as $l_1 = l(1-\lambda)$, $l_2 = l(1+\lambda)$, $\lambda \in [0,1]$ – which effectively means shifting one of the connections points around the loop as λ is changing – one arrives at the final resonance condition

$$\sin kl(1-\lambda)\sin kl(1+\lambda) - 4k^2\beta_1^{-1}(k)\beta_2^{-1}(k)\sin^2 kl$$
$$+k[\beta_1^{-1}(k)+\beta_2^{-1}(k)]\sin 2kl = 0\,,$$

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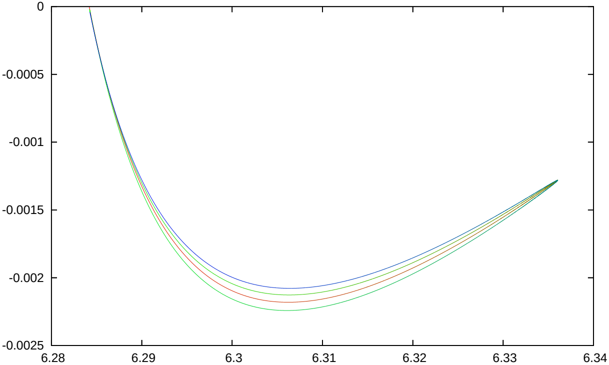
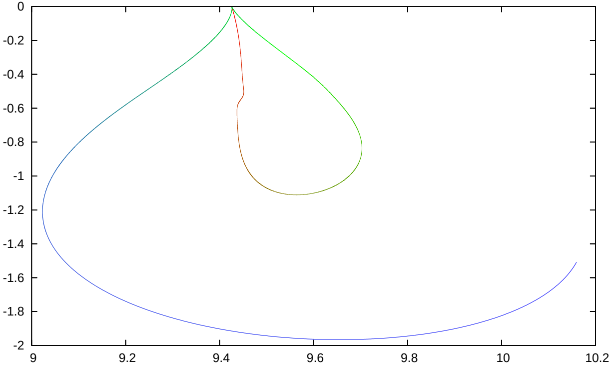
The condition can be solved numerically to find the resonance trajectories with respect to the variable λ.

A pole trajectory



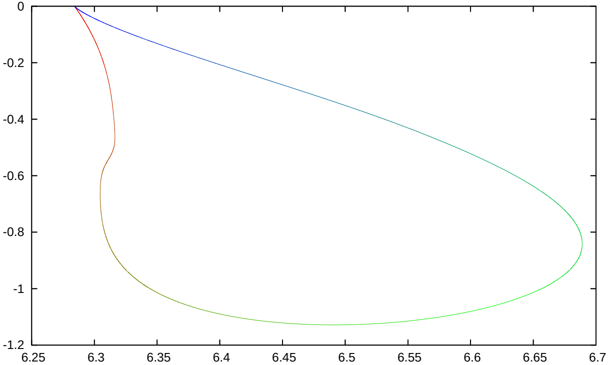
The trajectory of the resonance pole in the lower complex halfplane starting from $k_0 = 2\pi$ for the coefficients values $\alpha_1^{-1} = 1$, $\tilde{\alpha}_1^{-1} = -2$, $|\gamma_1|^2 = 1$, $\alpha_2^{-1} = 0$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_2|^2 = 1$, $n = 2$. The colour coding shows the dependence on λ changing from red ($\lambda = 0$) to blue ($\lambda = 1$).

Another pole trajectory



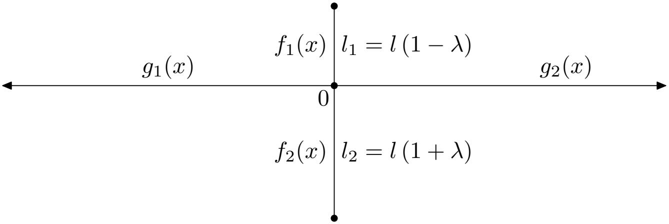
The trajectory of the resonance pole starting at $k_0 = 3\pi$ for the coefficients values $\alpha_1^{-1} = 1$, $\alpha_2^{-1} = 1$, $\tilde{\alpha}_1^{-1} = 1$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_1|^2 = |\gamma_2|^2 = 1$, $n = 3$. The colour coding is the same as in the previous picture.

One more pole trajectory



The trajectory of the resonance pole starting at $k_0 = 2\pi$ for the coefficients values $\alpha_1^{-1} = 1$, $\alpha_2^{-1} = 1$, $\tilde{\alpha}_1^{-1} = 1$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_1|^2 = 1$, $|\gamma_2|^2 = 1$, $n = 2$. The colour coding is the same as above.

Another example: a cross-shaped graph



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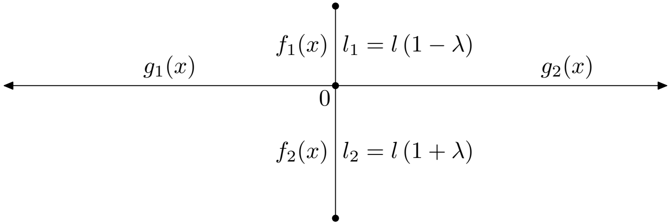


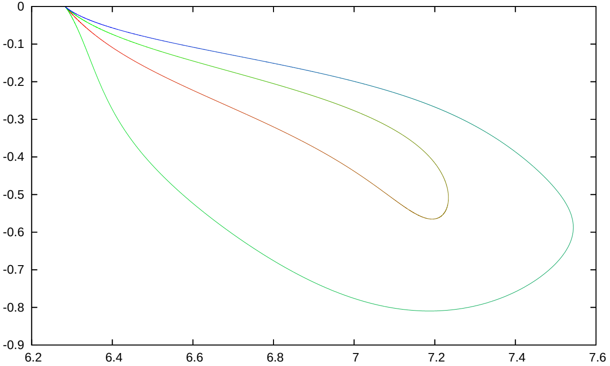
This time we restrict ourselves to the δ coupling as the boundary condition at the vertex and we consider Dirichlet conditions at the loose ends, i.e.

$$\begin{aligned} f_1(0) = f_2(0) = g_1(0) = g_2(0)\,, \\ f_1(l_1) = f_2(l_2) = 0\,, \\ \alpha f_1(0) = f_1'(0) + f_2'(0) + g_1'(0) + g_2'(0)\,. \end{aligned}$$

leading to the resonance condition

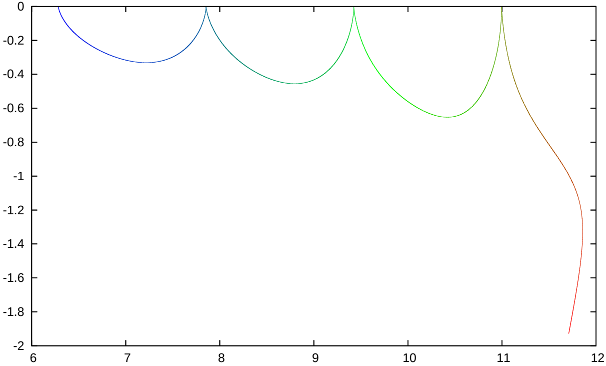
$$2k \sin 2kl + (\alpha - 2ik)(\cos 2kl\lambda - \cos 2kl) = 0$$

Pole trajectory



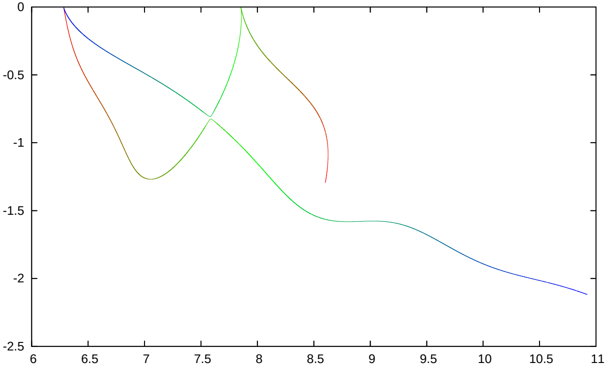
The trajectory of the resonance pole starting at $k_0 = 2\pi$ for the coefficients values $\alpha = 10$, $n = 2$. The colour coding is the same as in the previous figures.

Another pole trajectory: an anholonomy



The trajectory of the resonance pole for the coefficients values $\alpha = 1$, $n = 2$. The colour coding is the same as above.

More trajectories: an avoided crossing



The trajectories of two resonance poles for the coefficients values $\alpha = 2.596$, $n = 2$. We can see an avoided resonance crossing – the former eigenvalue "travelling from the left to the right" interchanges with the former resonance "travelling the other way" and ending up as an embedded eigenvalue. The colour coding is the same as above.

High-energy asymptotics

We begin form a deep insight by [Davies-Pushnitski'11] who looked into *high-energy asymptotics* of graph resonances. As usual *counting function* $N(R, F)$ is the number of zeros of $F(k)$ in the circle $\{k : |k| < R\}$ of given radius $R > 0$, algebraic multiplicities taken into account.

If the function F comes from resonance secular equation we count in this way *number of resonances* within the given circle. By resonances we mean here both the 'true' resonances and *embedded eigenvalues*

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Let us look how the situation looks like for graphs in which Kirchhoff is replaced by a *more general vertex couplings*

Recall the resonance condition

Denote $e_j^{\pm} := \mathrm{e}^{\pm ikl_j}$ and $e^{\pm} := \Pi_{j=1}^{N} e_j^{\pm}$, then the secular equation is

$$0 = \det\left\{\frac{1}{2}[(U-I) + k(U+I)]E_1(k) + \frac{1}{2}[(U-I) + k(U+I)]E_2 + k(U+I)E_3 \right.$$
$$\left. + (U-I)E_4 + [(U-I) - k(U+I)]\,\mathrm{diag}\,(0,\dots,0,I_{M\times M})\right\},$$

where $E_i(k) = \mathrm{diag}\,\left(E_i^{(1)}, E_i^{(2)}, \dots, E_i^{(N)}, 0, \dots, 0\right)$, $i = 1,2,3,4$, consists of N nontrivial 2×2 blocks

$$E_1^{(j)} = \begin{pmatrix} 0 & 0 \\ -ie_j^{+} & e_j^{+} \end{pmatrix},\; E_2^{(j)} = \begin{pmatrix} 0 & 0 \\ ie_j^{-} & e_j^{-} \end{pmatrix},\; E_3^{(j)} = \begin{pmatrix} i & 0 \\ 0 & 0 \end{pmatrix},\; E_4^{(j)} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

and the trivial $M \times M$ part.

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and the trivial $M\times M$ part.

Looking for zeros of the *rhs* we can employ a modification of a classical result on zeros of exponential sums [Langer'31]

Exponential sum zeros

Theorem (Langer'31)

Let $F(k) = \sum_{r=0}^{n} a_r(k)\,\mathrm{e}^{ik\sigma_r}$, *where* $a_r(k)$ *are rational functions of the complex variable* k *with complex coefficients, and the numbers* $\sigma_r \in \mathbb{R}$ *satisfy* $\sigma_0 < \sigma_1 < \cdots < \sigma_n$. *Suppose that* $\lim_{k\to\infty} a_0(k) \neq 0$ *and* $\lim_{k\to\infty} a_n(k) \neq 0$. *Then there are a compact* $\Omega \subset \mathbb{C}$, *real numbers* m_r *and positive* K_r, $r = 1, \dots, n$, *such that the zeros of* $F(k)$ *outside* Ω *lie in the logarithmic strips bounded by the curves* $-\mathrm{Im}\,k + m_r \log|k| = \pm K_r$ *and the counting function behaves in the limit* $R \to \infty$ *as*

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

Application of Langer theorem

We need the coefficients at $e^{\pm}$ in the resonance condition. Let us pass to the effective b.c. formulation,

$$0 = \det\Big\{\frac{1}{2}[(\tilde{U}(k)-I)+k(\tilde{U}(k)+I)]\tilde{E}_1(k)$$
$$+\frac{1}{2}[(\tilde{U}(k)-I)-k(\tilde{U}(k)+I)]\tilde{E}_2(k)+k(\tilde{U}(k)+I)\tilde{E}_3+(\tilde{U}(k)-I)\tilde{E}_4\Big\},$$

where $\tilde{E}_j$ are the nontrivial $2N\times 2N$ parts of the matrices E_j and I denotes the $2N\times 2N$ unit matrix

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\begin{aligned}
0 = \det \Big\{ & \frac{1}{2}[(\tilde{U}(k) - I) + k(\tilde{U}(k) + I)]\tilde{E}_1(k) \\
& + \frac{1}{2}[(\tilde{U}(k) - I) - k(\tilde{U}(k) + I)]\tilde{E}_2(k) + k(\tilde{U}(k) + I)\tilde{E}_3 + (\tilde{U}(k) - I)\tilde{E}_4 \Big\},
\end{aligned}
$$

where $\tilde{E}_j$ are the nontrivial $2N \times 2N$ parts of the matrices E_j and I denotes the $2N \times 2N$ unit matrix

By a direct computation we get

Lemma

The coefficients of senior and junior term, $e^{\pm}$ respectively, in the above equation are $\left(\frac{i}{2}\right)^N \det\left[(\tilde{U}(k) - I) \pm k(\tilde{U}(k) + I)\right]$

The resonance asymptotics

Theorem (Davies-E-Lipovský'10)

Consider a quantum graph (Γ, H_U) corresponding to Γ with finitely many edges and the coupling at vertices $\mathcal{X}_j$ given by unitary matrices U_j. The asymptotics of the resonance counting function as $R \to \infty$ is of the form

$$N(R, F) = \frac{2W}{\pi} R + \mathcal{O}(1)\,,$$

where W is the effective size of the graph. One always has

$$0 \leq W \leq V := \sum_{j=1}^{N} l_j.$$

Moreover $W < V$ (that is, graph is non-Weyl in the terminology of [Davies-Pushnitski'11] if and only if there exists a vertex where the corresponding energy dependent coupling matrix $\tilde{U}_j(k)$ has an eigenvalue $(1-k)/(1+k)$ or $(1+k)/(1-k)$.

Permutation invariant couplings

Now we apply the result to graphs with coupling invariant w.r.t. edge permutations. These are described by matrices $U_j = a_j J + b_j I$, where $a_j,\, b_j \in \mathbb{C}$ such that $|b_j| = 1$ and $|b_j + a_j \deg \mathcal{X}_j| = 1$; matrix J has all the entries equal to one.

Note that both the δ and δ'_{s} are particular cases of such a coupling.

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We need two simple auxiliary statements:

Lemma

The matrix $U = aJ_{n\times n} + bI_{n\times n}$ has $n-1$ eigenvalues b and one eigenvalue $na+b$. Its inverse is $U^{-1} = -\frac{a}{b(an+b)} J_{n\times n} + \frac{1}{b} I_{n\times n}$.

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Lemma

Let p internal and q external edges be coupled with b.c. given by $U = aJ_{(p+q)\times(p+q)} + bI_{(p+q)\times(p+q)}$. Then the energy-dependent effective matrix of the compact part is $\tilde{U}(k) = \frac{ab(1-k)-a(1+k)}{(aq+b)(1-k)-(k+1)} J_{p\times p} + bI_{p\times p}$.

Asymptotics in the permutation-symmetric case

Combining them with the above theorem we find easily that there are only two cases which exhibit non-Weyl asymptotics here:

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Theorem (Davies-E-Lipovský'10)

Let (Γ, H_U) be a quantum graph with permutation-symmetric coupling conditions at the vertices, $U_j = a_j J + b_j I$. Then it has non-Weyl asymptotics if and only if at least one of its vertices is balanced, $p = q$, and the coupling at this vertex is either

(a) $f_j = f_n, \quad \forall j, n \leq 2p, \quad \sum_{j=1}^{2p} f_j' = 0, \qquad i.e.\ U = \frac{1}{p} J_{2p\times 2p} - I_{2p\times 2p}$, or

(b) $f_j' = f_n', \quad \forall j, n \leq 2p, \quad \sum_{j=1}^{2p} f_j = 0, \qquad i.e.\ U = -\frac{1}{p} J_{2p\times 2p} + I_{2p\times 2p}$.

What can cause a non-Weyl asymptotics?

We will argue that (anti)Kirchhoff conditions at balanced vertices are too easy to decouple diminishing in this way effectively the graph size.

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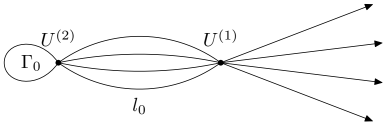

Consider the above graph with a balanced vertex $\mathcal{X}_1$ which connects p internal edges of the same length l_0 and p external edges with the coupling given by a unitary $U^{(1)} = aJ_{2p\times 2p} + bI_{2p\times 2p}$. The coupling to the rest of the graph, denoted as Γ_0, is described by a $q \times q$ matrix $U^{(2)}$, where $q \geq p$; needless to say such a matrix can hide different topologies of this part of the graph.

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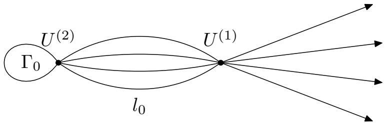

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Remark: The assumption about the same edge length is made for convenience only; we can always satisfy it by adding Kirchhhoff vertices

A simple unitary equivalence result

Proposition

Consider Γ be the the coupling given by arbitrary $U^{(1)}$ and $U^{(2)}$. Let V be an arbitrary unitary $p \times p$ matrix, $V^{(1)} := \mathrm{diag}\,(V, V)$ and $V^{(2)} := \mathrm{diag}\,(I_{(q-p)\times(q-p)}, V)$ be $2p \times 2p$ and $q \times q$ block diagonal matrices, respectively. Then H on Γ is unitarily equivalent to the Hamiltonian H_V on topologically the same graph with the coupling given by the matrices $[V^{(1)}]^{-1} U^{(1)} V^{(1)}$ and $[V^{(2)}]^{-1} U^{(2)} V^{(2)}$.

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We apply it to our system: let $U^{(1)} = aJ_{2p\times 2p} + bI_{2p\times 2p}$ at $\mathcal{X}_1$. We choose columns of W as an orthonormal set of eigenvectors of the $p \times p$ block $aJ_{p\times p} + bI_{p\times p}$, the first one being $\frac{1}{\sqrt{p}}(1, 1, \ldots, 1)^{\mathrm{T}}$. The transformed matrix $[V^{(1)}]^{-1} U^{(1)} V^{(1)}$ decouples into blocks connecting only pairs (v_j, g_j).

Implications for permutation-symmetric coupling

The first one corresponding to a *symmetrization* of all the u_j's and f_j's, leads to the 2×2 matrix $U_{2\times 2} = apJ_{2\times 2} + bI_{2\times 2}$, while the other lead to *separation of the corresponding internal and external edges* described by the Robin conditions, $(b-1)v_j(0) + i(b+1)v_j'(0) = 0$ and $(b-1)g_j(0) + i(b+1)g_j'(0) = 0$ for $j = 2, \dots, p$.

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The "overall" Kirchhoff/anti-Kirchhoff condition at $\mathcal{X}_1$ is transformed to the "line" Kirchhoff/anti-Kirchhoff condition in the subspace of permutation-symmetric functions, *reducing the graph size by l_0*. In all the other cases the point interaction corresponding to the matrix $apJ_{2\times 2} + bI_{2\times 2}$ is nontrivial, and consequently, *the graph size is preserved*.

Unbalanced non-Weyl graphs

On the other hand, in graphs with *unbalanced* vertices there are many cases of non-Weyl behaviour. To demonstrate it we employ another unitary equivalence trick based this time on the unitary transformation $W^{-1}UW$, where W is block diagonal with a nontrivial unitary $q \times q$ part W_4,

$$W = \begin{pmatrix} \mathrm{e}^{i\varphi} I_{p\times p} & 0 \\ 0 & W_4 \end{pmatrix}$$

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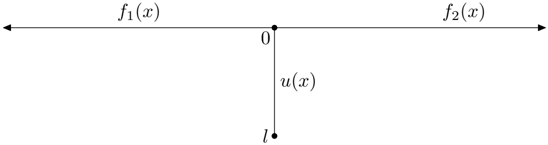
One can check easily the following claim:

Proposition

The operators H_U and $H_{W^{-1}UW}$ are unitarily equivalent, and as a consequence, the family of resonances of H_U does not change if the original coupling matrix U is replaced by $W^{-1}UW$.

Example: line with a stub



The Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$ on graph Γ consisting of two half-lines and one internal edge of length l. Its domain contains functions from $W^{2,2}(\Gamma)$ which satisfy

$$(U-I)\,(u(0), f_1(0), f_2(0))^{\mathrm{T}} + i(U+I)\,(u'(0), f_1'(0), f_2'(0))^{\mathrm{T}} = 0\,,$$
$$u(l) + cu'(l) = 0\,;$$

$f_i(x)$ referring to half-lines and $u(x)$ to the internal edge.

Example, continued

We start from the matrix $U_0 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \mathrm{e}^{i\psi} \end{pmatrix}$, describing one half-line separated from the rest of the graph. As mentioned above such a graph has non-Weyl asymptotics (obviously, it cannot have more than two resonances)

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Using $U_W = W^{-1}UW$ with $W = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r\mathrm{e}^{i\varphi_1} & \sqrt{1-r^2}\,\mathrm{e}^{i\varphi_2} \\ 0 & \sqrt{1-r^2}\,\mathrm{e}^{i\varphi_3} & -r\mathrm{e}^{i(\varphi_2+\varphi_3-\varphi_1)} \end{pmatrix}$

we arrive at a three-parameter family with the same resonances — *thus non-Weyl* — described by

$$U = \begin{pmatrix} 0 & r\mathrm{e}^{i\varphi_1} & \sqrt{1-r^2}\mathrm{e}^{i\varphi_2} \\ r\mathrm{e}^{-i\varphi_1} & (1-r^2)\mathrm{e}^{i\psi} & -r\sqrt{1-r^2}\mathrm{e}^{-i(-\psi+\varphi_1-\varphi_2)} \\ \sqrt{1-r^2}\mathrm{e}^{-i\varphi_2} & -r\sqrt{1-r^2}\mathrm{e}^{i(\psi+\varphi_1-\varphi_2)} & r^2\mathrm{e}^{i\psi} \end{pmatrix}$$

Effective size is a global property

One may ask whether there are geometrical rules that would quantify *separately* the effect of each balanced vertex on the asymptotics. The following *example* shows that this is not the case:

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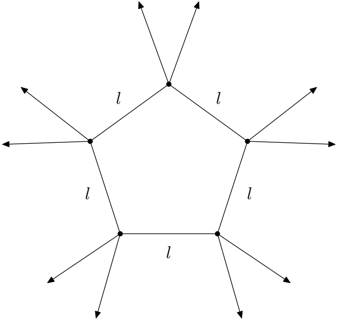

For a fixed integer $n \geq 3$ we start with a regular n-gon, each edge having length ℓ, and attach two semi-infinite leads to each vertex, so that each vertex is balanced; thus the *effective size W_n is strictly less than $V_n = n\ell$*.

Example, continued

Proposition

The effective size of the graph Γ_n is given by

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

Example, continued

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Sketch of the proof: We employ Bloch/Floquet decomposition of H w.r.t. the cyclic rotation group $\mathbb{Z}_n$. It leads to analysis of one segment with "quasimomentum" ω satisfying $\omega^n = 1$; after a short computation we find that H_ω has a resonance *iff*

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

Hence the effective size W_ω of the system of resonances of H_ω is $\ell/2$ if $\omega^2 + 1 \neq 0$ but it is zero if $\omega^2 + 1 = 0$. Now $\omega^2 + 1 = 0$ is not soluble if $\omega^n = 1$ and $n \neq 0$ mod 4, but it has two solutions if $n = 0$ mod 4. $\square$

Adding a magnetic field

Now the Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$ at the infinite leads and as $-(\mathrm{d}/\mathrm{d}x + iA_j(x))^2$ at the internal edges, where A_j is the tangent component of the vector potential.

Its domain consists of functions in $W^{2,2}(\Gamma)$ satisfying

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Using the local gauge transformation $\psi_j(x) \mapsto \psi_j(x)\mathrm{e}^{-i\chi_j(x)}$ with $\chi_j(x)' = A_j(x)$ one gets unitary equivalence to *free Hamiltonian* with the coupling

$$(U_A - I)\Psi + i(U_A + I)\Psi' = 0\,, \quad U_A := \mathcal{F}U\mathcal{F}^{-1}\,,$$

where $\mathcal{F} = \mathrm{diag}\,(1, \exp\,(i\Phi_1), \dots, 1, \exp\,(i\Phi_N), 1, \dots, 1)$ containing magnetic fluxes $\Phi_j = \int_0^{l_j} A_j(x)\,\mathrm{d}x$

Magnetic graph high-energy asymptotics

Theorem (E-Lipovský'11)

Let Γ be a quantum graph with N internal and M external edges and coupling given by a $(2N+M)\times(2N+M)$ unitary matrix U. Let Γ_V be obtained from Γ by replacing U by $V^{-1}UV$ where $\left(\begin{smallmatrix} V_1 & 0 \\ 0 & V_2 \end{smallmatrix}\right)$ is unitary block-diagonal matrix consisting of a $2N\times 2N$ block V_1 and an $M\times M$ block V_2. Then Γ_V has a non-Weyl resonance asymptotics iff Γ does.

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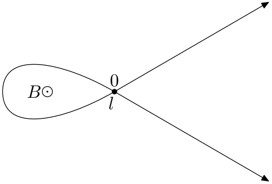
Corollary

Let Γ be a quantum graph with Weyl resonance asymptotics. Then Γ_A has also the Weyl asymptotics for any profile of the magnetic field.

Example: the effective size can be affected

The magnetic field can change, though, the effective size, as the following example shows:



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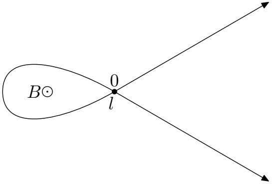

This (Kirchhoff) graph is non-Weyl for $A = 0$, and thus for any A. The resonance condition is easily found to be

$$-2\cos\Phi + \mathrm{e}^{-ikl} = 0\,,$$

where $\Phi = Al$ is the loop flux. For $\Phi = \pm\pi/2 \pmod \pi$, odd multiples of a quarter of the flux quantum 2π, the l-independent term disappears. The effective size of the graph is then zero; it is straightforward to see that in the present case there are *no resonances at all*.

Generalized graphs

Let us finally mention briefly a generalization of quantum graphs, with "edges" of different dimensions – some speak in this connection about *hedgehog manifolds*

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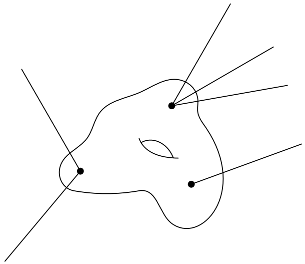

Generalized graphs

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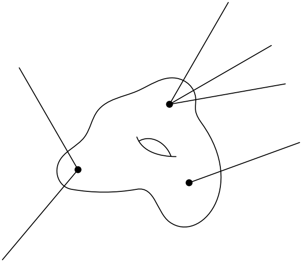

For simplicity we consider the case with a single manifold part only

The formalism

We generalize here slightly [E-Tater-Vaněk'01, [Brüning-Geyler'03], [Brüning-E-Geyler'03] where each lead was supposed to be attached at a different point.

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Let Ω be a compact Riemannian manifold of dimension $d = 2, 3$ with metric g from which we make Γ by attaching $M = \sum_j n_j$ halflines at points $x_j \in \Omega$. The state space is

$$\mathcal{H} = L^2(\Omega, \mathrm{d}g) \bigoplus_{i=1}^{M} L^2(\mathbb{R}_+^{(i)})$$

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In the manifold part, let H_0 be Laplace-Beltrami operator acting on $C_0^\infty(\Omega)$ as $-g^{-1/2}\partial_r(g^{1/2}\partial_r)$ with suitable b.c. if Ω has a boundary; by H_0' we denote it restriction to functions $\{f(x) : f(x_j) = 0\}$ which is a symmetric operator with deficiency indices (n, n).

Formalism, continued

Let further H_i' be restriction of the Laplacian on ith halfline to functions from $C_0^\infty(\mathbb{R}_+^{(i)})$. The operator

$$H' = H_0' \oplus H_1' \oplus \cdots \oplus H_M'$$

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To construct self-adjoint extensions of the operator H' we need (generalized) boundary values. $f \in D((H_0')^*)$ can be expanded near x_j as $f(x) = c_j(f)F_0(x,x_j) + d_j(f) + \mathcal{O}(r(x,x_j))$, where

$$F_0(x,x_j) = \begin{cases} -\frac{q_2(x,x_j)}{2\pi} \ln r(x,x_j) & d=2 \\ \frac{q_3(x,x_j)}{4\pi} (r(x,x_j))^{-1} & d=3 \end{cases}$$

here q_2, q_3 are continuous functions of x with $q_i(x_j,x_j) = 1$ and $r(x,x_j)$ denotes the geodesic distance between x and x_j

Self-adjoint extensions

Using the expansion we write the boundary values as

$$\Psi = (d_1(f), \dots, d_n(f), f_1(0), \dots, f_M(0))^{\mathrm{T}}\,,$$
$$\Psi' = (c_1(f), \dots, c_n(f), f_1'(0), \dots, f_M'(0))^{\mathrm{T}}\,,$$

and describe any s-a extension of H' by the conditions

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

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This covers all the self-adjoint extensions of H' including those allowing 'hopping' between vertices. We are interested in *local* ones only; they are characterized by *block-diagonal* matrices U which does not couple different points x_i and x_j.

Effective coupling on the manifold

As in the quantum graph case we can study resonances on hedgehog manifolds replacing external leads by an effective energy-dependent coupling at the points $x_j \in \Omega$ as follows

$$(\tilde{U}_j(k) - 1)d_j(f) + i(\tilde{U}_j(k) + 1)c_j(f) = 0$$

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where $\tilde{U}_j(k) \in \mathbb{C}$ is easily seen to be given by

$$\tilde{U}_j(k) = U_{1j} - (1-k)U_{2j}[(1-k)U_{4j} - (k+1)I]^{-1}U_{3j}$$

and U_{1j} denotes top-left entry of U_j, U_{2j} the rest of the first row, U_{3j} the rest of the first column and U_{4j} is $n_j \times n_j$ part corresponding to the coupling between the halflines attached to the manifold.

In a sense we have replaced again the leads by *k-dependent point interactions* on the manifold Ω itself.

Scattering and resolvent resonances

We have a natural framework to study Ω as a geometric scatterer taking solution of Schrödinger equation on the j-th lead as $a_j(k)\mathrm{e}^{-ikx} + b_j(k)\mathrm{e}^{ikx}$

A caveat: Since the leads are *positive* halflines, our S-matrix convention differs from the one used in 1D scattering:

$$S(k)^{-1} = S(-k) = S^*(\bar{k})$$

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By *scattering resonance* we mean a pole of the scattering matrix, more precisely, the (complex) energy at which some of its entries has a pole

By *resolvent resonance* we mean a pole in *analytical continuation* of $(H-k^2)^{-1}$. As before we can use *exterior complex scaling* on the edges turning resonances into ev's of the *non-selfadjoint operator* $H_\theta := U_\theta H U_\theta^{-1}$

Resonance equivalence

Lemma

Let $H\big|_\Omega f(x,k) = kf(x,k)$ *hold for* $k^2 \notin \sigma(H_0)$, *then* f *is as a linear combination of Green's functions of* H_Ω,

$$f(x,k) = \sum_{j=1}^{n} c_j G(x, x_j; k)$$

Proof modifies the argument of [Kiselev'97].

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Proof modifies the argument of [Kiselev'97].

Using this result we can prove

Theorem (E-Lipovský'11)

Consider the lower complex halfplane of momentum, $\mathrm{Im}\, k < 0$ and $k^2 \notin \mathbb{R}$. There is a scattering resonance in k_0 iff there is a resolvent resonance in k_0, and the algebraic multiplicities of resonances defined in both ways coincide.

Proof sketch

Using the lemma and $a_j(k)\mathrm{e}^{-ikx} + b_j(k)\mathrm{e}^{ikx}$ as Ansatz on the leads one arrives at the condition

$$A(k_0)\mathbf{a} + B(k_0)\mathbf{b} + C(k_0)\mathbf{c} = 0\,,$$

where A, B are $(P+M)\times M$ matrices, C is $(P+M)\times P$ matrix, P is the number of internal parameters of the geometric scatterer and M is the number of halflines.

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If $k_0^2 \notin \mathbb{R}$ the columns of $C(k_0)$ are linearly independent, otherwise k_0 would have to be an eigenvalue. A rearrangement allows us to express $\mathbf{c}$; substituting it to the remaining conditions we get

$$\tilde{A}(k_0)\mathbf{a} + \tilde{B}(k_0)\mathbf{b} = 0$$

with $\tilde{A}(k_0)$ and $\tilde{B}(k_0)$ being $M\times M$ matrices.

Proof sketch, continued

If $\det \tilde{A}(k_0) = 0$ holds than there is a solution with $\mathbf{b} = 0$ and k_0 is an eigenvalue of H with $\mathrm{Im}\, k_0 < 0$, however, this contradicts the selfadjointness of H. Hence by Cramer's rule the scattering resonances are given by the condition $\det \tilde{B}(k) = 0$.

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The solution $a_j(k)\mathrm{e}^{-ikx}$ on the j-th halfline is taken by U_θ into an exponentially growing one if $\mathrm{Im}\, k_0 < 0$ and $\mathrm{Im}\, \theta > 0$, while $b_j(k)\mathrm{e}^{ikx}$ becomes square integrable. Hence solving the eigenvalue problem for $\mathbf{H}_\theta$ one needs to find solutions with $\mathbf{a} = 0$. This leads again to the condition $\det \tilde{B}(k) = 0$ proving thus the claim. $\square$

Explicit resonance condition

The above lemma allows us to express the boundary values using expansion of deficiency subspace elements,

$$f(x_i,k) = c_i F_0(x_i,x_i) + \sum_{j\neq i}^{n} c_j F_0(x_i,x_j) + \sum_{j=1}^{n} c_j F_1(x_i,x_j;k) + \sum_{j=1}^{n} c_j R(x_i,x_j;k)$$

where $R(x_i,x_j;k)$ is $\mathcal{O}(r(x_i,x_j))$

Let $\tilde{U}(k) = \mathrm{diag}\,(\tilde{U}_1(k),\dots,\tilde{U}_n(k),)$; definition of $\tilde{U}_j(k)$ shows that $\tilde{U}(k)$ diverges at at most M values of k. We define

$$Q_0(k) = \begin{cases} G(x_i,x_j;k) & i\neq j \\ F_1(x_i,x_i;k) & i=j \end{cases}$$

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The resonance condition then reads as follows

$$\det\left[(\tilde{U}(k)-I)Q_0(k) + i(\tilde{U}(k)+I)\right] = 0$$

Magnetic 'hedgehogs': an example

Due to the 2D nature of the manifold no 'non-Weyl' surprises are expected. However, we are going to illustrate that even for generalized graphs a magnetic field *can kill all 'true' resonances of the system.*

We consider Ω being a disc with Dirichlet boundary to which a lead is attached, the field is zero outside z-axis being of *Aharonov-Bohm type* passing through the centre of the disc

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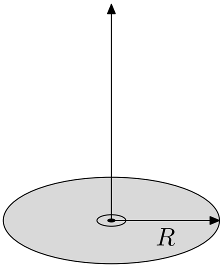

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$$\dot{H}_\alpha \binom{u}{f} = \begin{pmatrix} -\frac{\partial^2 u}{\partial r^2} - \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\left(i\frac{\partial}{\partial \varphi} - \alpha\right)^2 u \\ -f'' \end{pmatrix}$$

defined on functions $\binom{u}{f}$ with $u \in \mathcal{H}^2_{\mathrm{loc}}(B_R(0))$ satisfying conditions $u(0,\varphi) = u(R,\varphi) = 0$ and $f \in \mathcal{H}^2_{\mathrm{loc}}(\mathbb{R}^+)$ s.t. $f(0) = f'(0) = 0$

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We take $\alpha \in (0,1)$ for the value of the magnetic flux since integer values can be easily gauged away

Disc-and-lead example, continued

By partial-wave decomposition we have to analyze the operators

$$\dot{h}_{\alpha,m}\phi = -\frac{\mathrm{d}^2\phi}{\mathrm{d}r^2} + \frac{(m+\alpha)^2 - 1/4}{r^2}\phi\,;$$

for $\alpha \neq 0$ the components with $m = 0, -1$ can be coupled

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We employ the following boundary values

$$\begin{aligned}
\Phi_1^{-1}(\psi) &= \sqrt{\pi}\lim_{r\to 0}\frac{r^{1-\alpha}}{2\pi}\int_0^{2\pi} u(r,\varphi)\mathrm{e}^{i\varphi}\mathrm{d}\varphi\,,\\
\Phi_2^{-1}(\psi) &= \sqrt{\pi}\lim_{r\to 0}\frac{r^{-1+\alpha}}{2\pi}\left[\int_0^{2\pi} u(r,\varphi)\mathrm{e}^{i\varphi}\mathrm{d}\varphi - 2\pi r^{-1+\alpha}\Phi_{-1}^{1}(\psi)\right],\\
\Phi_1^{0}(\psi) &= \sqrt{\pi}\lim_{r\to 0}\frac{r^{\alpha}}{2\pi}\int_0^{2\pi} u(r,\varphi)\mathrm{d}\varphi\,,\\
\Phi_2^{0}(\psi) &= \sqrt{\pi}\lim_{r\to 0}\frac{r^{-\alpha}}{2\pi}\left[\int_0^{2\pi} u(r,\varphi)\mathrm{d}\varphi - 2\pi r^{-\alpha}\Phi_1^{0}(\psi)\right],\\
\Phi_1^{\mathrm{h}}(\psi) &= f(0)\,, \quad \Phi_2^{\mathrm{h}}(\psi) = f'(0)\,.
\end{aligned}$$

Disc-and-lead example, continued

If the resonances should be absent one has to get rid, e.g., of the potential for the $m = 0$ function, hence we choose $\alpha = 1/2$ and the coupling conditions

$$(U - I)\Phi_1(\psi) + i(U + I)\Phi_2(\psi) = 0\,,$$

where $\Phi_a(\psi) = (\Phi_a^{\mathrm{h}}, \Phi_a^0, \Phi_a^{-1})^{\mathrm{T}}$ for $a = 1, 2$, and

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$$U = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \mathrm{e}^{i\rho} \end{pmatrix},$$

i.e. the nonradial part ($m = -1$) of the disc function is coupled to neither of the other two, while the radial part ($m = 0$) is coupled to the halfline via Kirchhoff condition.

Disc-and-lead example, concluded

The generalized eigenfunction allowed by these conditions has $u(r) = r^{-1/2}(c \sin k(R-r))$ and $f(x) = c\sqrt{\pi} \sin k(x+R)$

Hence for any $k \notin \mathbb{R}$ and $c \neq 0$ the function f contains a nontrivial part of the wave e^{-ikx}, however, a resolvent resonance must have the asymptotics e^{ikx} only. This allows us to conclude:

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Proposition (E-Lipovský'13)

The described system has no true resonances for the indicated disc-lead coupling and the magnetic flux $\alpha = \frac{1}{2}$.

The results discussed in the talk come from

- [DEL10] E.B. Davies, P.E., J. Lipovský: Non-Weyl asymptotics for quantum graphs with general coupling conditions, *J. Phys. A: Math. Theor.* **43** (2010), 474013
- [DP11] E.B. Davies, A. Pushnitski: Non-Weyl resonance asymptotics for quantum graphs, *Analysis and PDE* **4** (2011), 729-756
- [EL10] P.E., J. Lipovský: Resonances from perturbations of quantum graphs with rationally related edges, *J. Phys. A: Math. Theor.* **43** (2010), 105301
- [EL11] P.E., J. Lipovský: Non-Weyl resonance asymptotics for quantum graphs in a magnetic field, *Phys. Lett.* **A375** (2011), 805-807
- [EP13] P.E., O. Post: Approximation of quantum graph vertex couplings by scaled Schrödinger operators on thin branched manifolds , *Commun. Math. Phys.* (2013), to appear; `arXiv:1205.5129`
- [EL13] P.E., J. Lipovský: Resonances on hedgehog manifolds, *Acta Polytechnica* (2013), to appear; `arXiv:1302.5269`

It remains to say

Thank you for your attention!