Quantum graphs: geometric perturbations, resonances, and Weyl asymptotics

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Talk overview

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- *Geometric perturbation:* eigenvalues in gaps and resonances in a model of “bent” chain graph
- *Another geometric perturbation:* resonances due to edge rationality violation in graphs with leads
- *High-energy asymptotics* of resonances: Weyl and non-Weyl behaviour, and when each of them occurs

Introduction: the quantum graph concept

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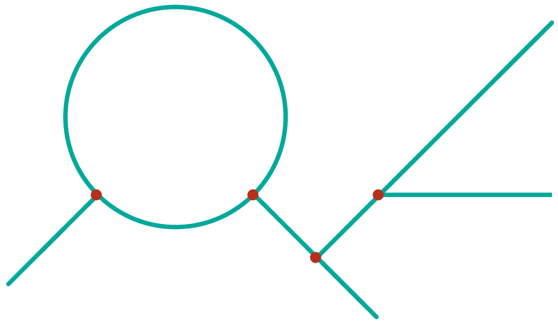
The concept extends, however, to graphs of *arbitrary shape*



Hamiltonian: $-\frac{\partial^2}{\partial x_j^2} + v(x_j)$
on graph edges,
boundary conditions at vertices

and what is important, it became *practically important* after experimentalists learned in the last two decades to fabricate tiny graph-like structure for which this is a good model

Remarks

- There are many graph-like systems based on *semiconductor* or *metallic* materials, *carbon nanotubes*, etc. The dynamics can be also simulated by *microwave network* built of optical cables – see [Hul et al.'04]

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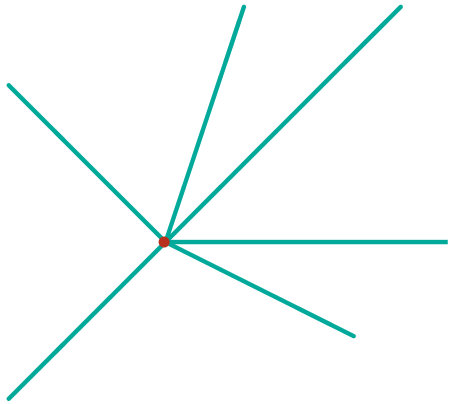
- Graphs can support also *Dirac operators*, see [Bulla-Trenckler'90], [Bolte-Harrison'03], and many recent applications to *graphene* and its derivates
- The graph literature is extensive; a good up-to-date reference are proceedings of the recent semester AGA Programme at INI Cambridge

Vertex coupling



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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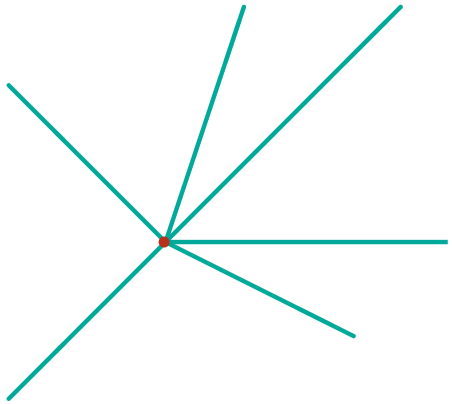

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Since it is second-order, the boundary condition involve $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$ being of the form

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

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

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

Unique 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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One can derive them modifying the argument used in [Fülöp-Tsutsui'00] for generalized point interactions, $n = 2$

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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- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *δ_s' coupling*

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

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

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Ask about relations between the geometry of Γ and spectral properties of a Schrödinger operator supported by Γ. An interpretation needed: think of Γ as of a subset of $\mathbb{R}^n$ with the *geometry inherited from the ambient space*

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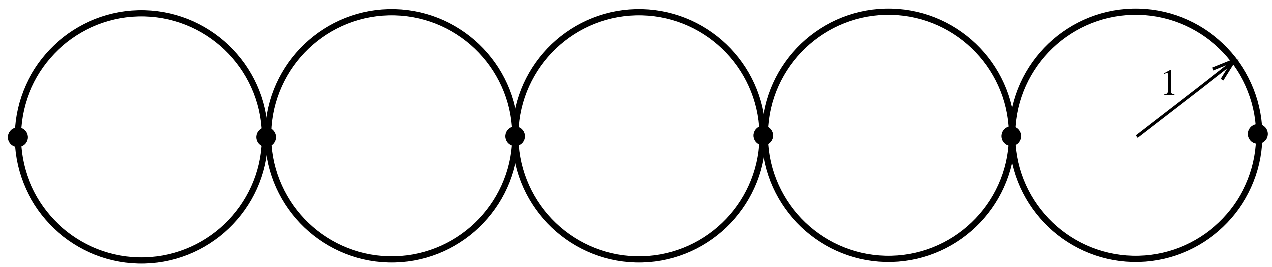
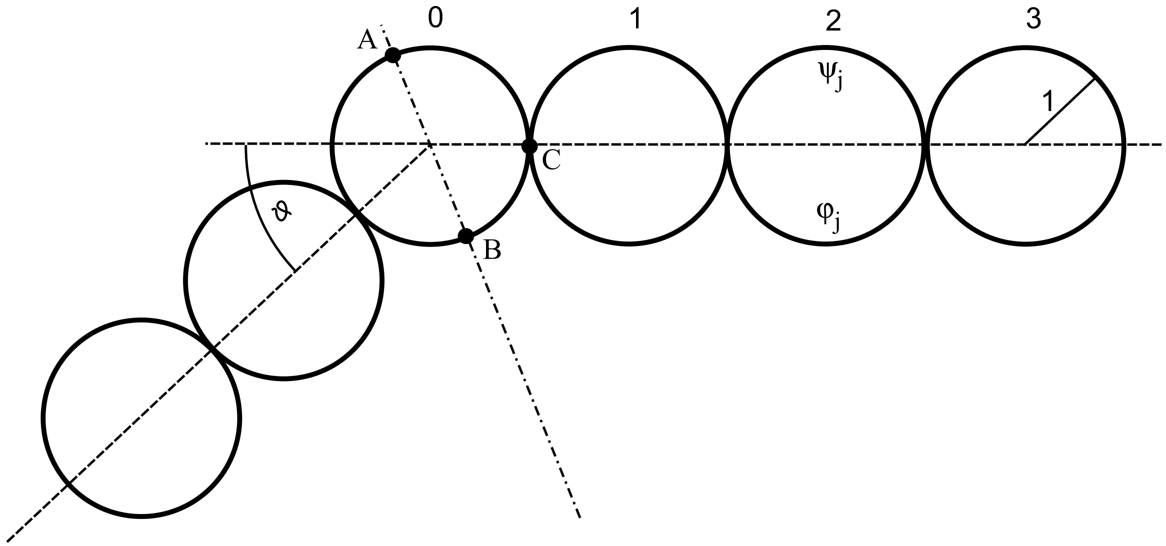
A simple model: analyze the *influence of a “bending” deformation* on a a “chain graph” which exhibits a one-dimensional periodicity



Without loss of generality we assume unit radii; the rings are connected by the δ-*coupling* of a strength $\alpha \neq 0$

Bending the chain

We will suppose that the chain is deformed as follows



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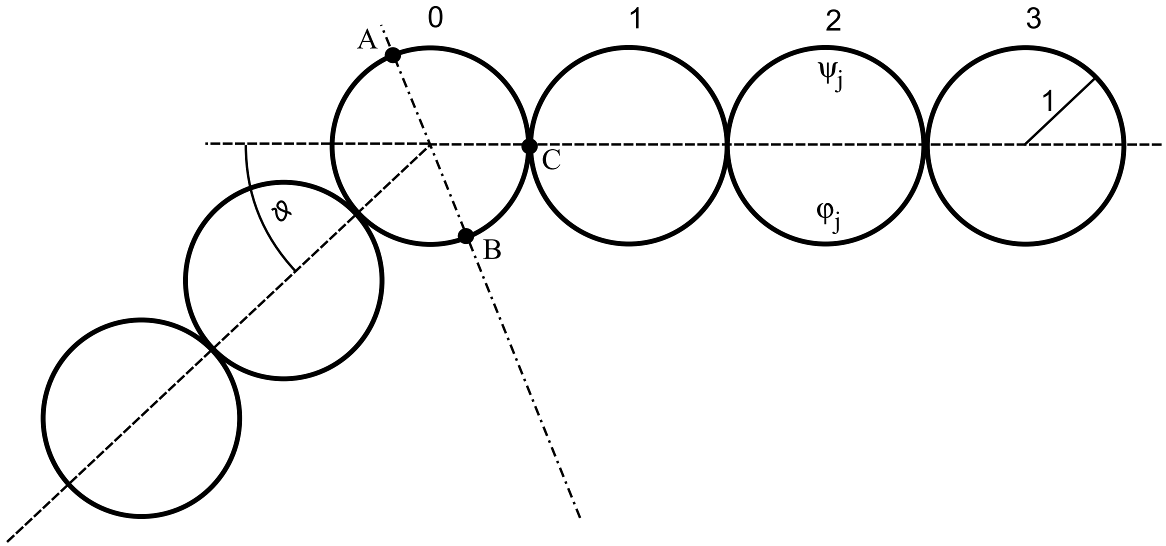
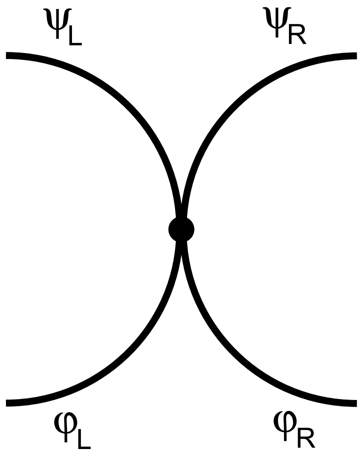


Our aim is to show that

- the band spectrum of the straight Γ is preserved
- there are *bend-induced eigenvalues*, we analyze their behavior with respect to model parameters
- the bent chain exhibits also *resonances*

An infinite periodic chain

The “straight” chain Γ_0 can be treated as a periodic system analyzing the spectrum of the elementary cell



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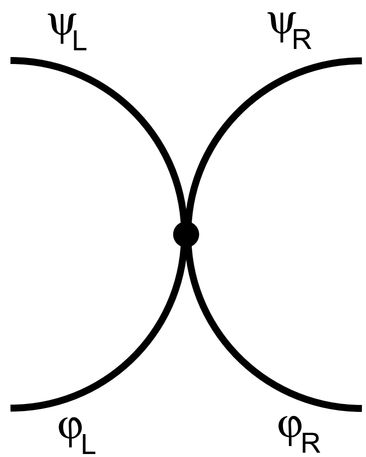

with Floquet-Bloch boundary conditions with the phase $\mathrm{e}^{2\mathrm{i}\theta}$

This yields the condition

$$\mathrm{e}^{2\mathrm{i}\theta} - \mathrm{e}^{\mathrm{i}\theta}\left(2\cos k\pi + \frac{\alpha}{2k}\sin k\pi\right) + 1 = 0$$

Straight chain spectrum

A straightforward analysis leads to the following conclusion:

Proposition: $\sigma(H_0)$ consists of *infinitely degenerate eigenvalues* equal to n^2 with $n \in \mathbb{N}$, and *absolutely continuous spectral bands* such that

If $\alpha > 0$, then every spectral band is contained in $(n^2, (n+1)^2]$ with $n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, and its upper edge coincides with the value $(n+1)^2$.

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If $\alpha < 0$, then in each interval $[n^2, (n+1)^2)$ with $n \in \mathbb{N}$ there is exactly one band with the lower edge n^2. In addition, there is a band with the lower edge (the overall threshold) $-\kappa^2$, where κ is the largest solution of

$$\left| \cosh \kappa\pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa\pi}{\kappa} \right| = 1$$

Straight chain spectrum

Proposition, cont'd: The upper edge of this band depends on α. If $-8/\pi < \alpha < 0$, it is k^2 where k solves

$$\cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k} = -1$$

in $(0,1)$. On the other hand, for $\alpha < -8/\pi$ the upper edge is negative, $-\kappa^2$ with κ being the smallest solution of the condition, and for $\alpha = -8/\pi$ it equals zero.

Finally, $\sigma(H_0) = [0, +\infty)$ holds if $\alpha = 0$.

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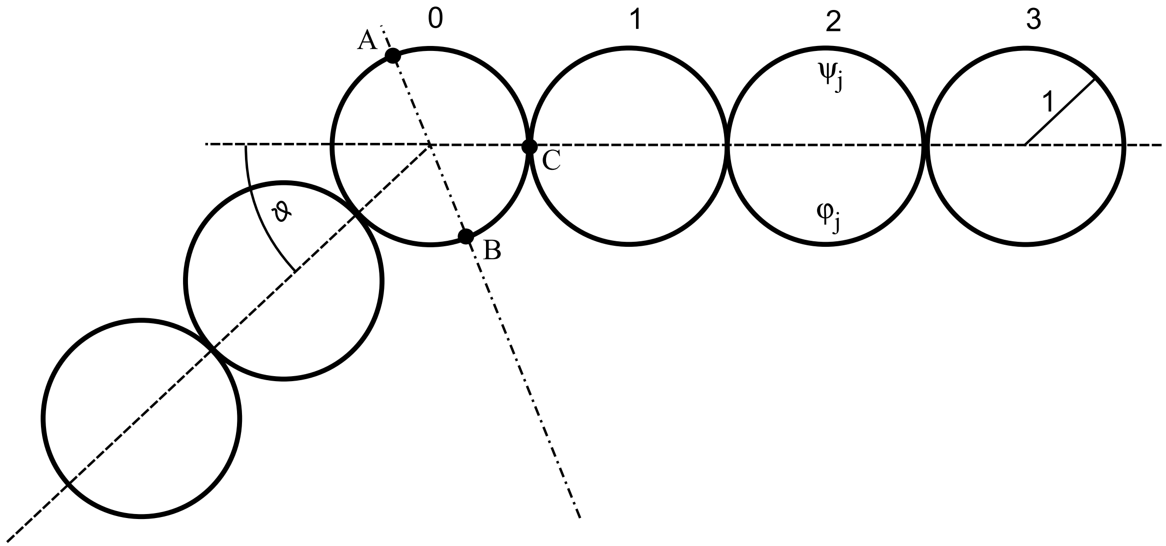
Let us add a couple of *remarks*:

- The bands correspond to *Kronig-Penney model* with the coupling $\frac{1}{2}\alpha$ instead of α, in addition one has here the *infinitely degenerate point spectrum*
- It is also an example of *gaps coming from decoration*

The bent chain spectrum

Now we pass to the bent chain denoted as Γ_ϑ:



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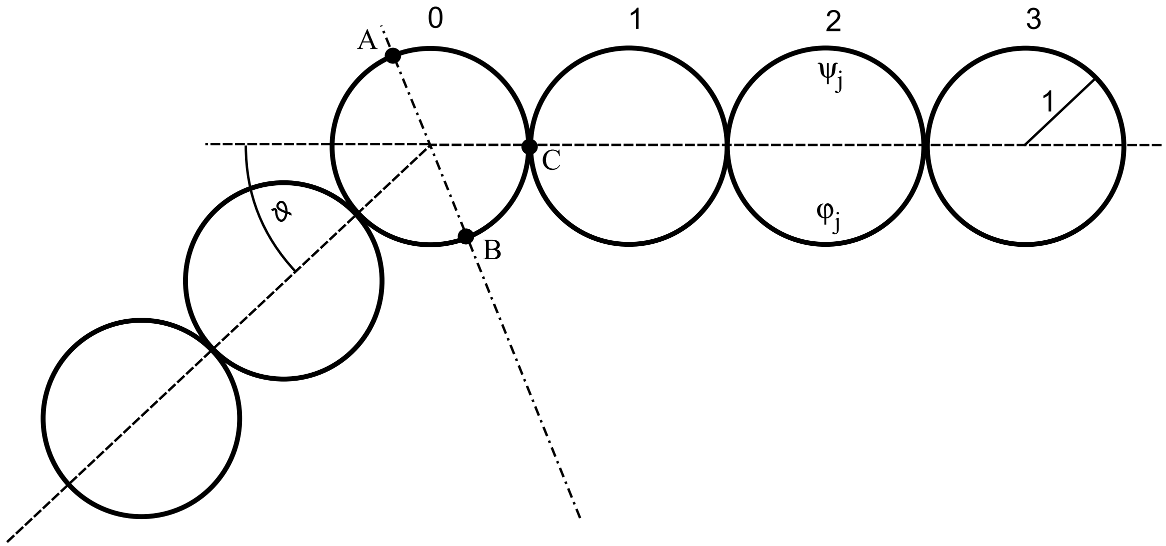

Since Γ_ϑ has mirror symmetry, the operator H_ϑ can be reduced by parity subspaces into a direct sum of an even part, H^+, and odd one, H^-; we drop mostly the subscript ϑ

Equivalently, we analyze the half-chain with *Neumann* and *Dirichlet* conditions at the points A, B, respectively

Eigenfunction components

At the energy k^2 they are are linear combinations of $\mathrm{e}^{\pm \mathrm{i}kx}$,

$$\begin{aligned} \psi_j(x) &= C_j^+ \mathrm{e}^{\mathrm{i}kx} + C_j^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0,\pi]\,, \\ \varphi_j(x) &= D_j^+ \mathrm{e}^{\mathrm{i}kx} + D_j^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0,\pi] \end{aligned}$$

for $j \in \mathbb{N}$. On the other hand, for $j = 0$ we have

$$\begin{aligned} \psi_0(x) &= C_0^+ \mathrm{e}^{\mathrm{i}kx} + C_0^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in \left[\frac{\pi-\vartheta}{2}, \pi\right] \\ \varphi_0(x) &= D_0^+ \mathrm{e}^{\mathrm{i}kx} + D_0^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in \left[\frac{\pi+\vartheta}{2}, \pi\right] \end{aligned}$$

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There are δ-couplings in the points of contact, i.e.

$$\psi_j(0) = \varphi_j(0)\,, \quad \psi_j(\pi) = \varphi_j(\pi)\,, \quad \text{and}$$

$$\psi_j(0) = \psi_{j-1}(\pi)\,; \quad \psi_j'(0) + \varphi_j'(0) - \psi_{j-1}'(\pi) - \varphi_{j-1}'(\pi) = \alpha \cdot \psi_j(0)$$

Transfer matrix

Using the above relations we get for all $j \geq 2$

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = \underbrace{\begin{pmatrix} \left(1+\frac{\alpha}{4\mathrm{i}k}\right)\mathrm{e}^{\mathrm{i}k\pi} & \frac{\alpha}{4\mathrm{i}k}\mathrm{e}^{-\mathrm{i}k\pi} \\ -\frac{\alpha}{4\mathrm{i}k}\mathrm{e}^{\mathrm{i}k\pi} & \left(1-\frac{\alpha}{4\mathrm{i}k}\right)\mathrm{e}^{-\mathrm{i}k\pi} \end{pmatrix}}_{M} \cdot \begin{pmatrix} C_{j-1}^+ \\ C_{j-1}^- \end{pmatrix},$$

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To have eigenvalues, one eigenvalue of M has to be *less than one* (they satisfy $\lambda_1 \lambda_2 = 1$); this happens *iff*

$$\left| \cos k\pi + \frac{\alpha}{4k} \sin k\pi \right| > 1\,;$$

recall that reversed inequality characterizes spectral bands

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Remark: By general arguments, σ_{ess} is preserved, and there are at most two eigenvalues in each gap

Spectrum of H^+

Combining the above with the Neumann condition at the mirror axis we get the spectral condition in this case,

$$\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}$$

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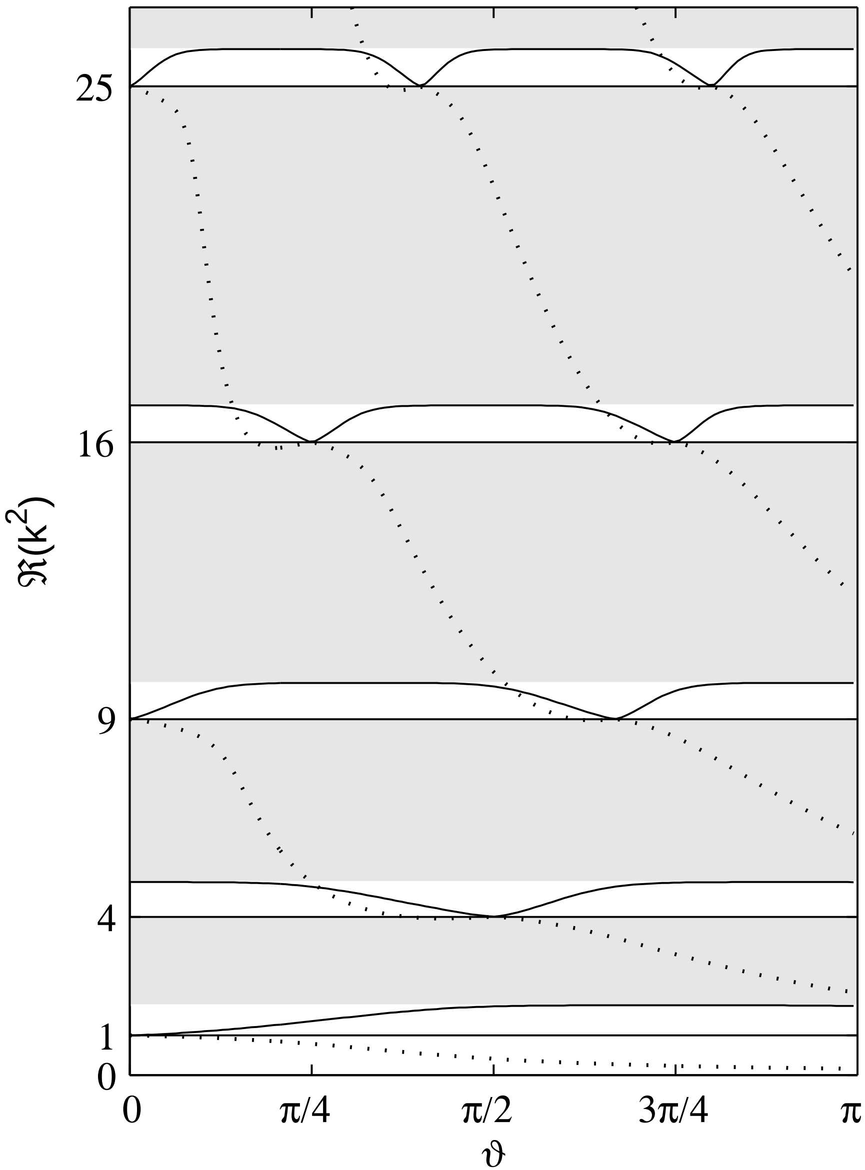
After a tiresome but straightforward analysis one arrives then at the following conclusion:

Proposition: If $\alpha \geq 0$, then H^+ has no negative eigenvalues. On the other hand, for $\alpha < 0$ the operator H^+ has at least one negative eigenvalue which lies under the lowest spectral band and above the number $-\kappa_0^2$, where κ_0 is the (unique) solution of $\kappa \cdot \tanh \kappa\pi = -\alpha/2$

Spectrum of H^+ for $\alpha = 3$



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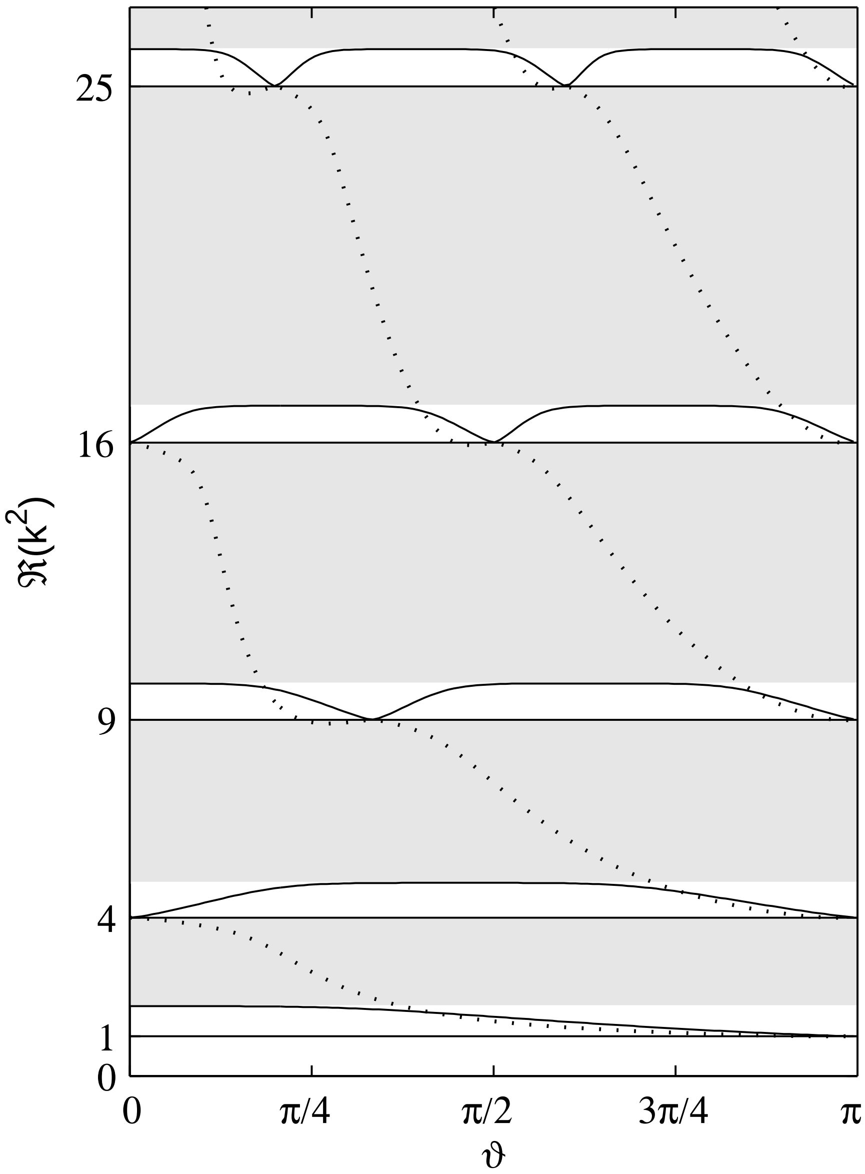
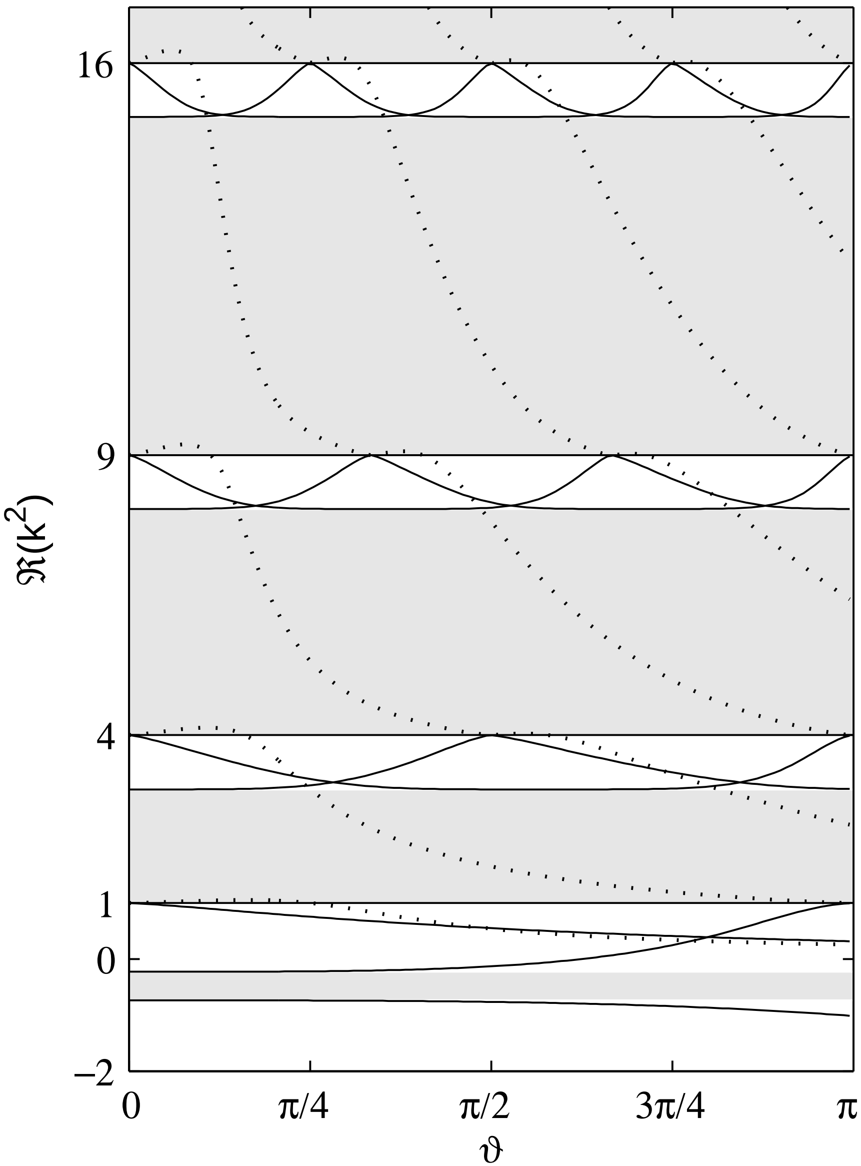
Summarizing, for each of the operators $H^{\pm}$ there is at least one eigenvalue in every spectral gap closure. It can lapse into a band edge n^2, $n \in \mathbb{N}$, and thus be in fact absent. The ev's of H^+ and H^- may coincide, becoming a single ev of multiplicity two; this happens only if

$$k \cdot \tan k\pi = \frac{\alpha}{2}$$

Spectrum of H^- for $\alpha = 3$



$\sigma(H)$ for attractive coupling, $\alpha = -3$



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The above eigenvalue curves are not the only solutions of the spectral condition. There are also *complex solutions* representing *resonances* of the bent-chain system

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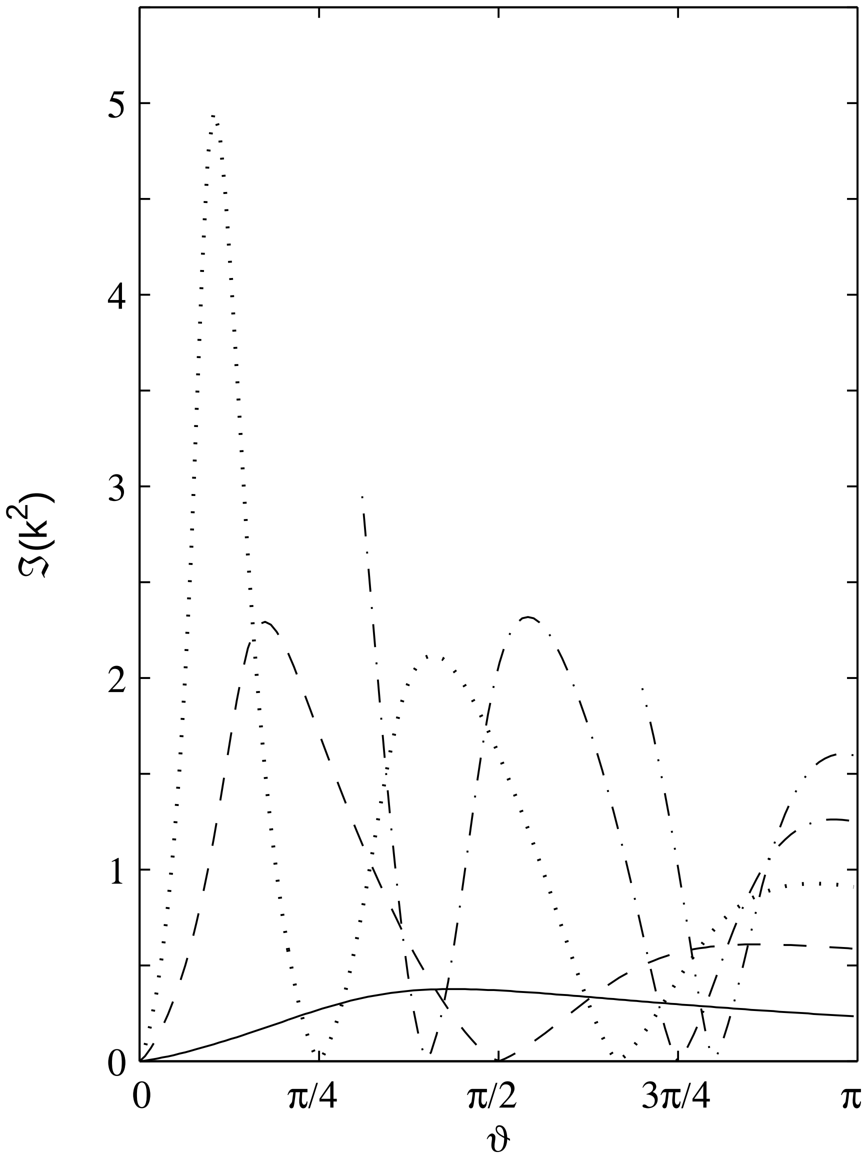
In the above pictures their real parts are drawn as functions of ϑ by dashed lines.

A further analysis of the spectral condition gives

Proposition: The eigenvalue and resonance curves for H^+ are *analytic* everywhere except at $(\vartheta, k) = (\frac{n+1-2\ell}{n}\pi, n)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}_0$, $\ell \leq \left[\frac{n+1}{2}\right]$. Moreover, the real solution in the n-th spectral gap is given by a function $\vartheta \mapsto k$ which is *real-analytic*, except at the points $\frac{n+1-2\ell}{n}\pi$. Similar claims can be made for the odd part for H^-.

Imaginary parts of H^+ resonances, $\alpha = 3$



More on the angle dependence

For simplicity we take H^+ only, the results for H^- are analogous. Ask about the behavior of the curves at the points whe they touch bands and where eigenvalues and resonances may cross

If $\vartheta_0 := \frac{n+1-2\ell}{n}\pi > 0$ is such a point we find easily that in is vicinity we have

$$k \approx k_0 + \sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\,|\vartheta - \vartheta_0|^{4/3}$$

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However, H^+ has an eigenvalue near $\vartheta_0 = 0$ also in the gaps adjacent to even numbers, when the curve starts at $(0, k_0)$ for k_0 solving $|\cos k\pi + \frac{\alpha}{4k}\sin k\pi| = 1$ in $(n, n+1)$, n even

Even threshold behavior

Proposition: Suppose that $n \in \mathbb{N}$ is even and k_0 is as described above, i.e. k_0^2 is the right endpoint of the spectral gap adjacent to n^2. Then the behavior of the solution in the vicinity of $(0, k_0)$ is given by

$$k = k_0 - C_{k_0,\alpha} \cdot \vartheta^4 + \mathcal{O}(\vartheta^5)\,,$$

where $C_{k_0,\alpha} := \frac{k_0^2}{8\pi} \cdot \left(\frac{\alpha}{4}\right)^3 (k_0\pi + \sin k_0\pi)^{-1}$

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Remark: Notice that the fourth-power is the same as for the ground state of a *slightly bent Dirichlet tube* despite the fact that the dynamics is completely different in the two cases

Second problem concerning resonances

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- Geometric perturbations of such graphs may turn the embedded eigenvalues into resonances

Preliminaries

Consider a graph Γ with 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 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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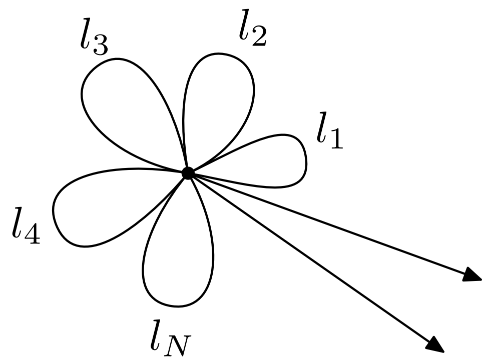
The Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$ on each link satisfying the boundary conditions

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

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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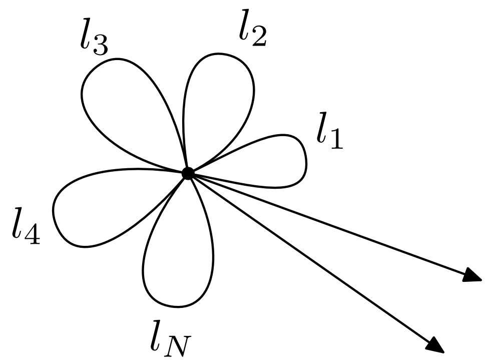

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The coupling is described by "big", $(2N+M)\times(2N+M)$ unitary block diagonal matrix U consisting of blocks U_j as follows,

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

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

Equivalence of 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-graph part: we set $f_j(x) = a_j \sin kx + b_j \cos kx$ on the internal edges

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

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

Scattering resonances

In this case we choose 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 $d = Sc$.

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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 resonance definitions, cont

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, $\det S^{-1} = 0$, if

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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 the finite 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

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

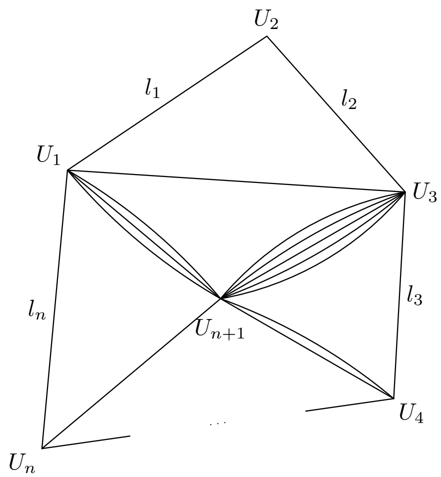
where the corresponding coupling matrix

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

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

Embedded ev's for commensurate edges

Suppose that the compact part contains a loop consisting of rationally related edges



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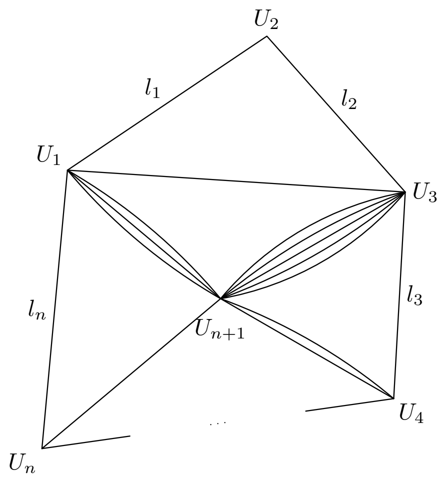

Then the graph Hamiltonian can have eigenvalues *with compactly supported eigenfunctions*; they are embedded in the continuum corresponding to external semiinfinite edges

Embedded eigenvalues

Theorem [E-Lipovský'10]: Let Γ consist of a single vertex and N finite edges emanating from this vertex and ending at it, with the coupling described by a $2N \times 2N$ unitary matrix U. Let the lengths of the first n edges be integer multiples of a positive real number l_0. If the rectangular $2N \times 2n$ matrix

$$M_{\text{even}} = \begin{pmatrix} u_{11} & u_{12}-1 & u_{13} & u_{14} & \cdots & u_{1,2n-1} & u_{1,2n} \\ u_{21}-1 & u_{22} & u_{23} & u_{24} & \cdots & u_{2,2n-1} & u_{2,2n} \\ u_{31} & u_{32} & u_{33} & u_{34}-1 & \cdots & u_{3,2n-1} & u_{3,2n} \\ u_{41} & u_{42} & u_{43}-1 & u_{44} & \cdots & u_{4,2n-1} & u_{4,2n} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ u_{2N-1,1} & u_{2N-1,2} & u_{2N-1,3} & u_{2N-1,4} & \cdots & u_{2N-1,2n-1} & u_{2N-1,2n} \\ u_{2N,1} & u_{2N,2} & u_{2N,3} & u_{2N,4} & \cdots & u_{2N,2n-1} & u_{2N,2n} \end{pmatrix}$$

has rank smaller than $2n$ then the spectrum of the corresponding Hamiltonian $H = H_U$ contains eigenvalues of the form $\epsilon = 4m^2\pi^2/l_0^2$ with $m \in \mathbb{N}$ and the multiplicity of these eigenvalues is at least the difference between $2n$ and the rank of M_{even}.

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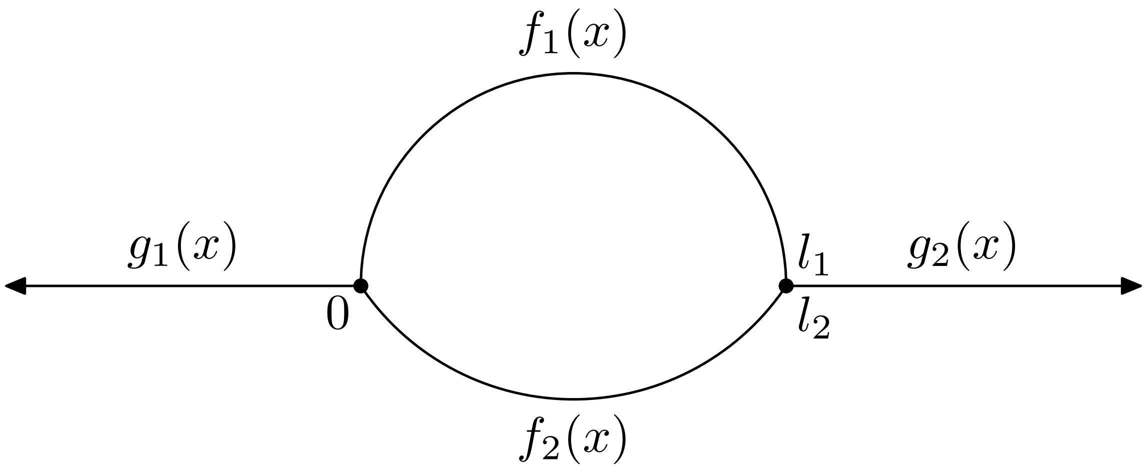
Example: a loop with two leads



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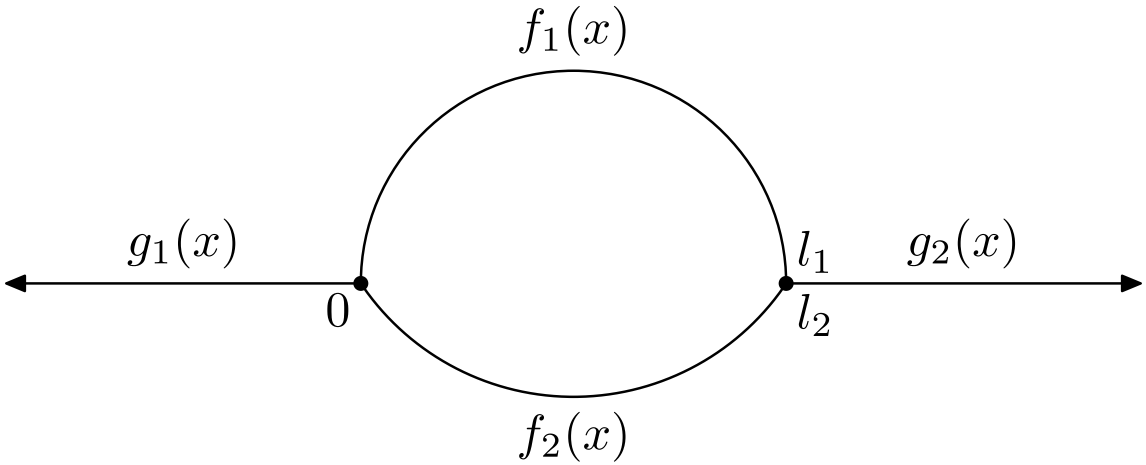

The setting is as above, the b.c. at the nodes are

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

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

$$\sin kl(1-\lambda)\sin kl(1+\lambda) - 4k^2\beta_1^{-1}(k)\beta_2^{-1}(k)\sin^2 kl$$

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

where $\beta_i^{-1}(k) := \alpha_i^{-1} + \frac{ik|\gamma_i|^2}{1-ik\tilde{\alpha}_i^{-1}}$.

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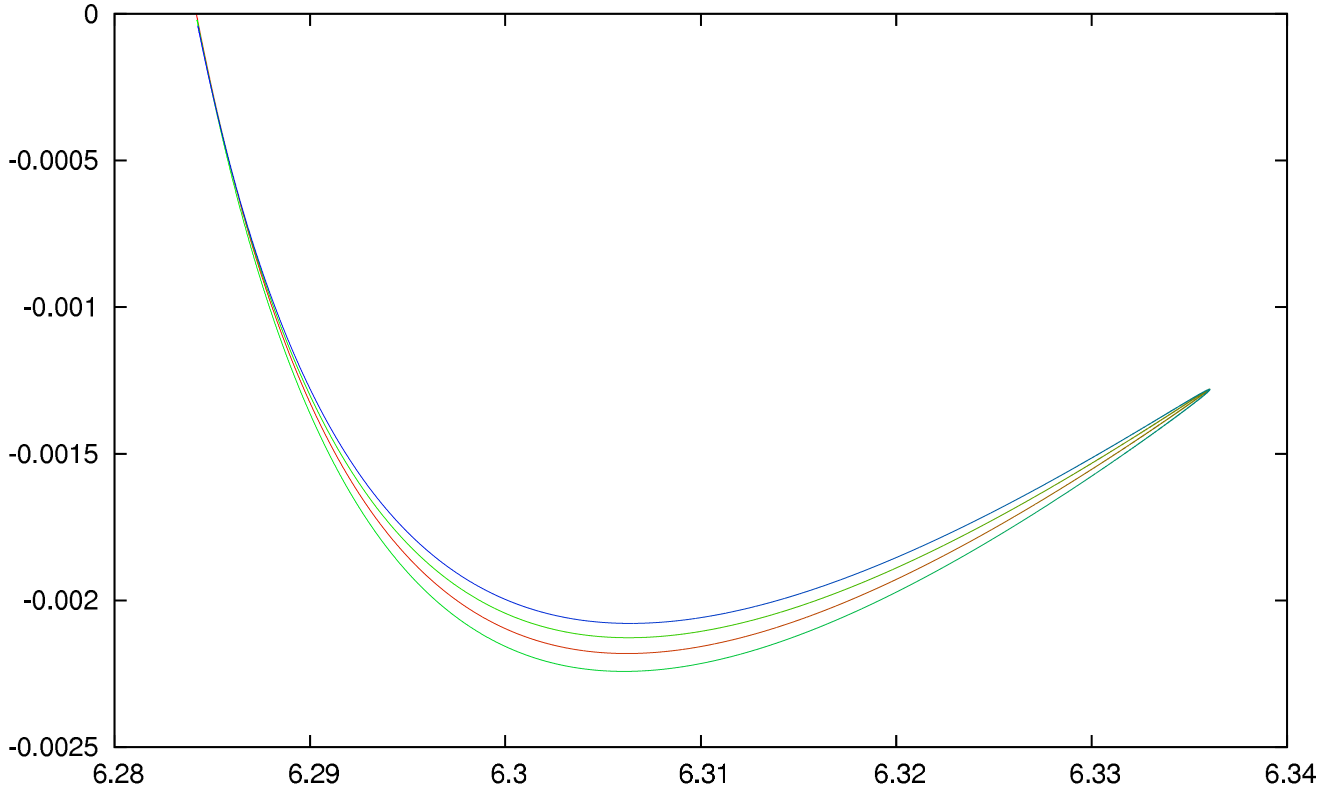
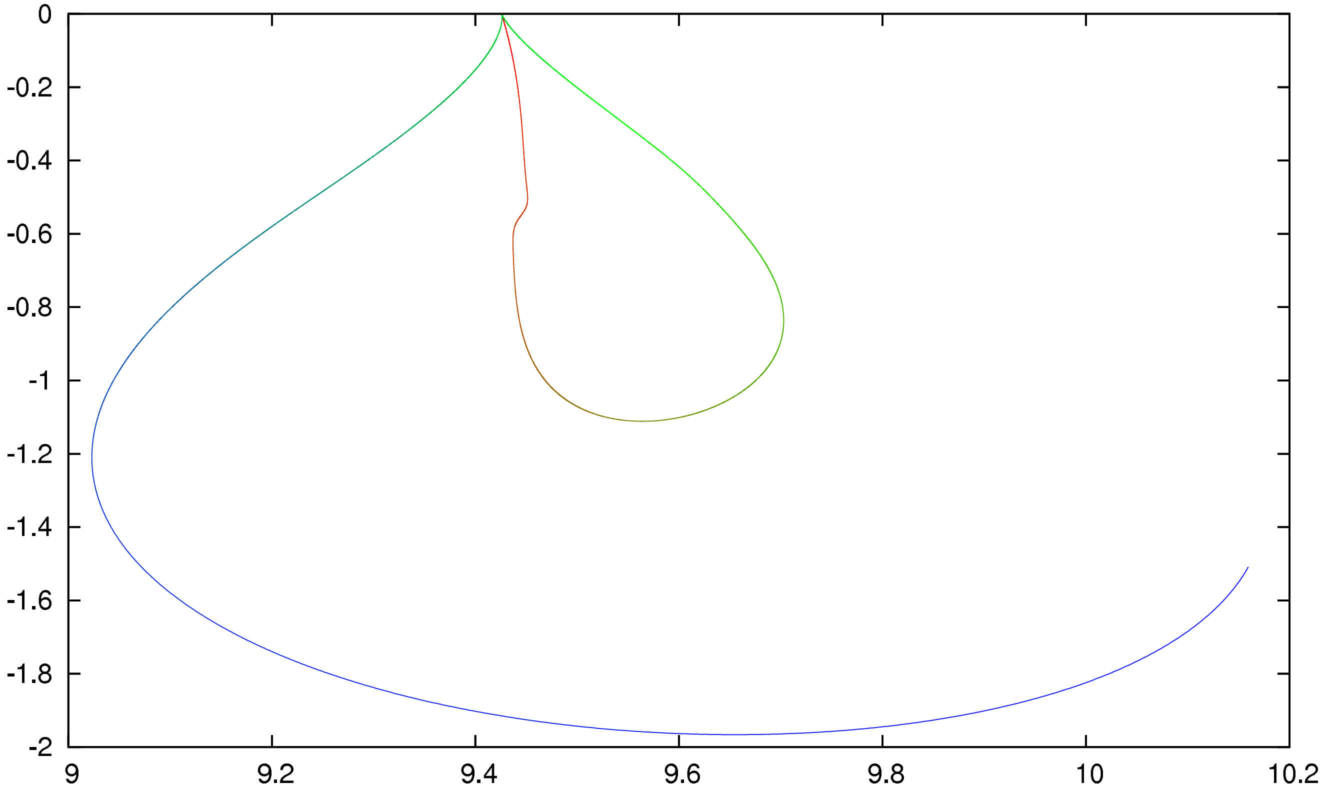
The condition can be solved numerically to find the resonance trajectories with respect to the variable λ.

Pole trajectory



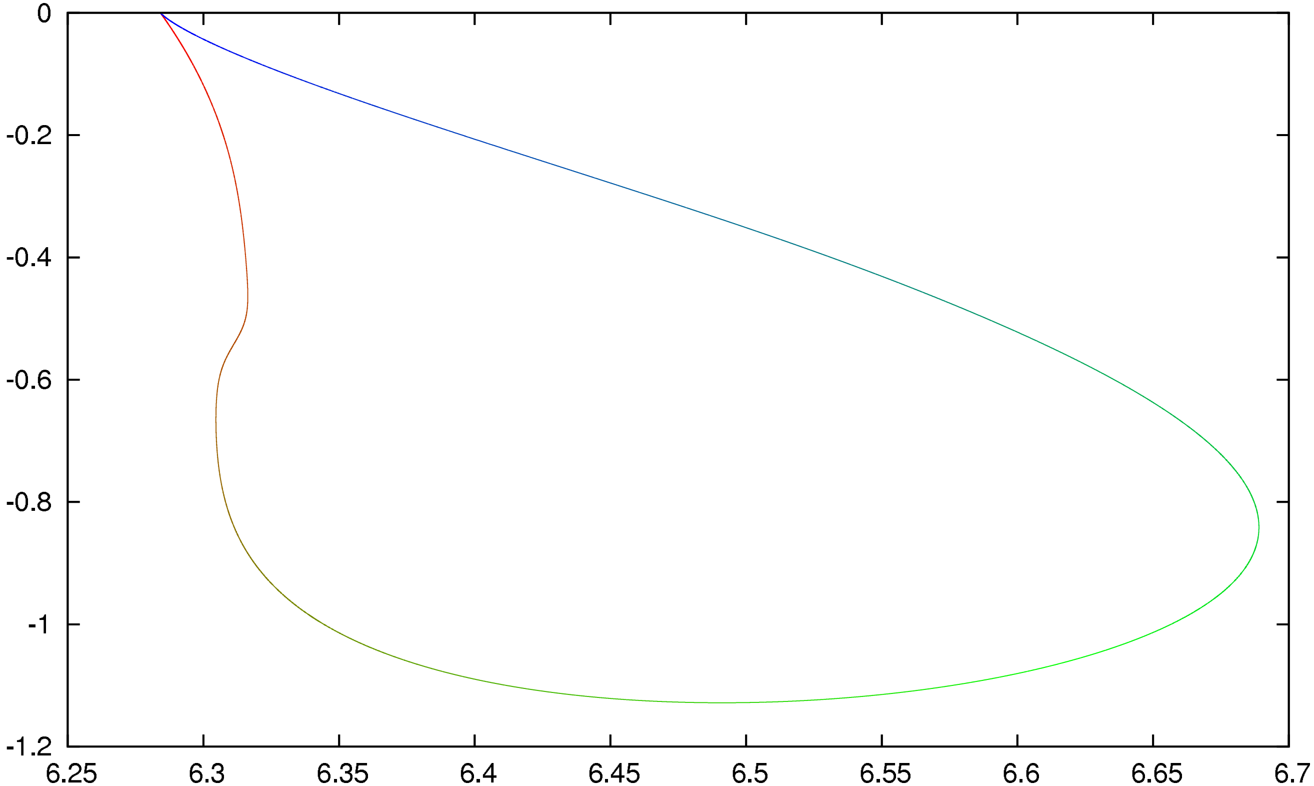
The trajectory of the resonance pole in the lower complex halfplane starting from $k_0 = 2\pi$ for the coefficients values $\alpha_1^{-1} = 1$, $\tilde{\alpha}_1^{-1} = -2$, $|\gamma_1|^2 = 1$, $\alpha_2^{-1} = 0$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_2|^2 = 1$, $n = 2$. The colour coding shows the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

Pole trajectory



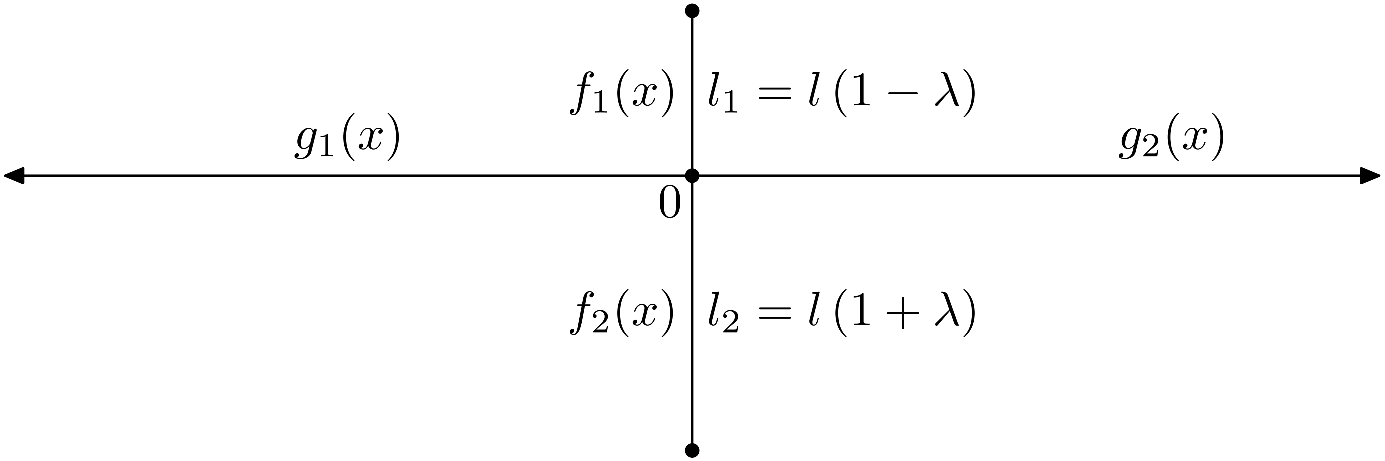
The trajectory of the resonance pole starting at $k_0 = 3\pi$ for the coefficients values $\alpha_1^{-1} = 1$, $\alpha_2^{-1} = 1$, $\tilde{\alpha}_1^{-1} = 1$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_1|^2 = |\gamma_2|^2 = 1$, $n = 3$. The colour coding is the same as in the previous picture.

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.

Example: a cross-shaped graph



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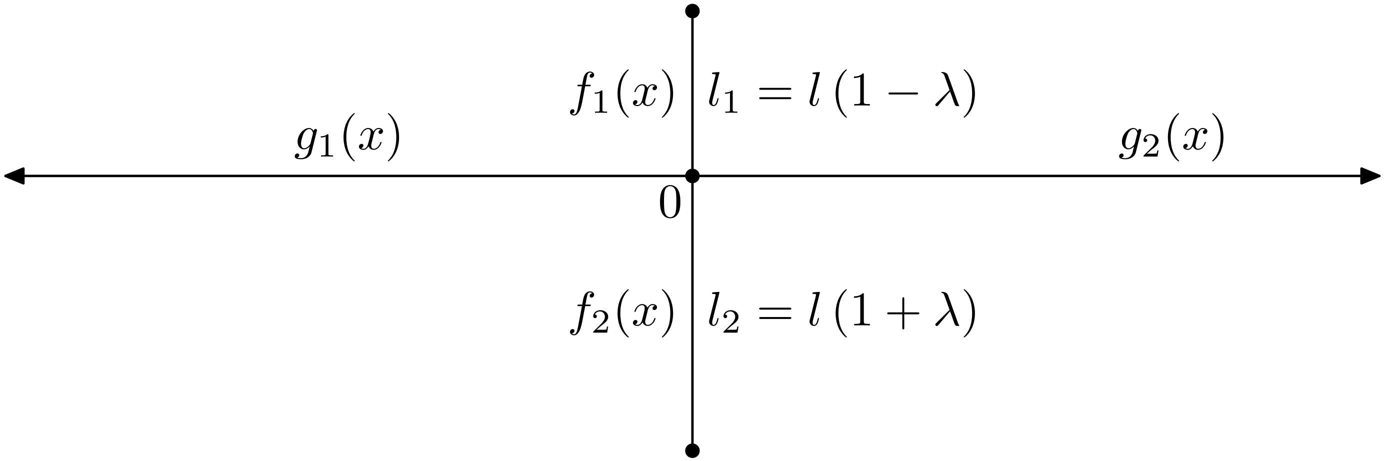


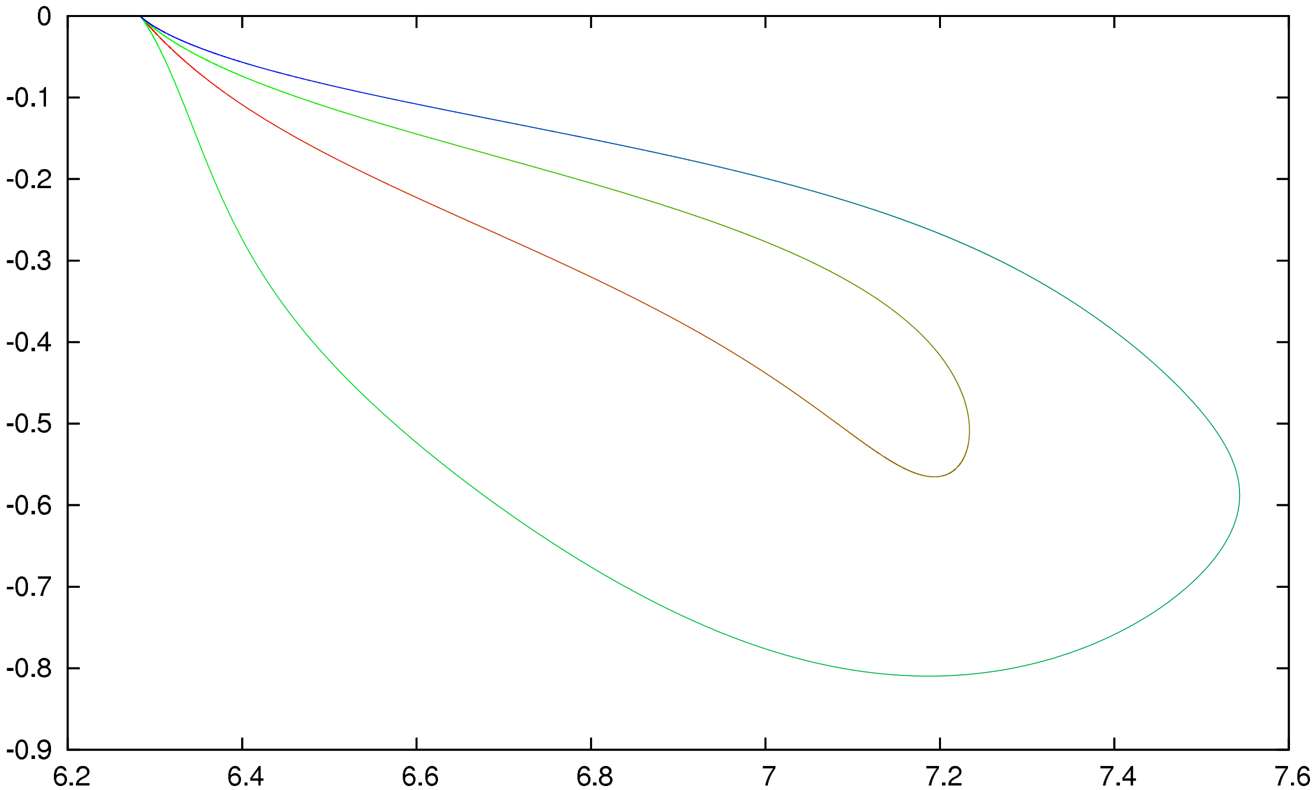
This time we restrict ourselves to the δ coupling as the boundary condition at the vertex and we consider Dirichlet conditions at the loose ends, i.e.

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

leading to the resonance condition

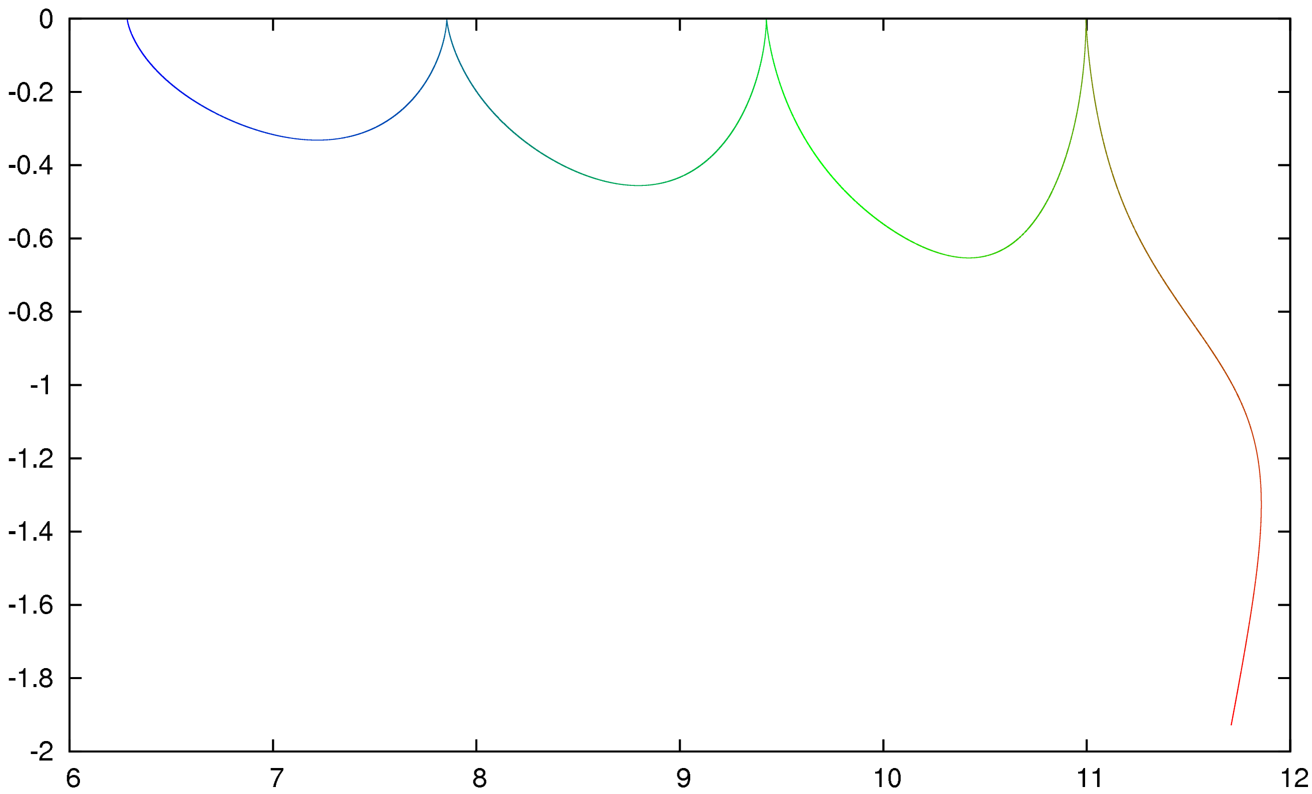
$$2k\sin 2kl + (\alpha - 2ik)(\cos 2kl\lambda - \cos 2kl) = 0$$

Pole trajectory



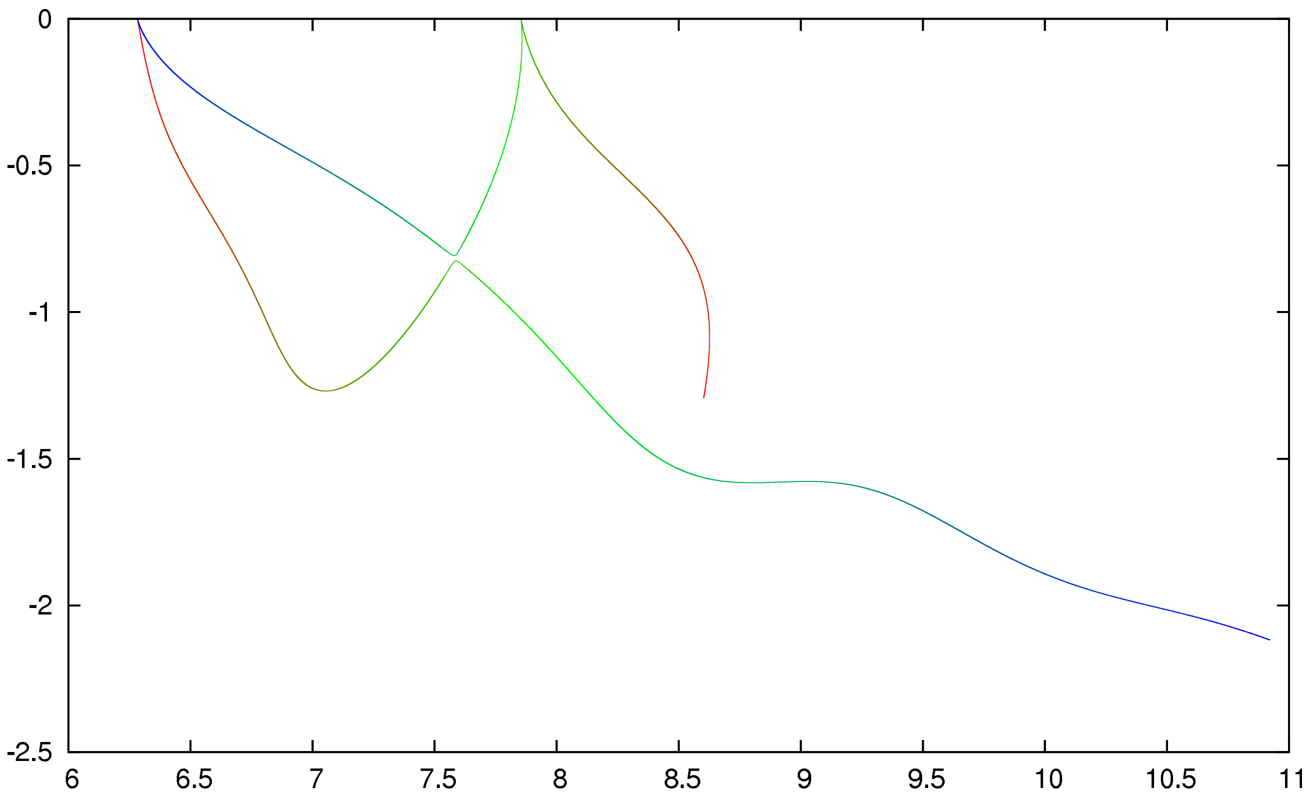
The trajectory of the resonance pole starting at $k_0 = 2\pi$ for the coefficients values $\alpha = 10$, $n = 2$. The colour coding is the same as in the previous figures.

Pole trajectory



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

Pole trajectory



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.

Multiplicity preservation

In a similar way resonances can be generated in the general case. What is important, nothing is “lost”:

Theorem [E-Lipovský’10]: Let Γ have N finite edges of lengths l_i, M infinite edges, and the coupling given by $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$, where U_4 refers to infinite edge coupling. Let k_0 satisfying $\det\left[(1-k_0)U_4 - (1+k_0)I\right] \neq 0$ be a pole of the resolvent $(H - \lambda\,\mathrm{id})^{-1}$ of a multiplicity d. Let Γ_ε be a geometrically perturbed quantum graph with edge lengths $l_i(1+\varepsilon)$ and the same coupling. Then there is $\varepsilon_0 > 0$ s.t. for all $\vec{\varepsilon} \in \mathcal{U}_{\varepsilon_0}(0)$ the sum of multiplicities of the resolvent poles in a sufficiently small neighbourhood of k_0 is d.

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Theorem [E-Lipovský’10]: Let Γ have N finite edges of lengths l_i, M infinite edges, and the coupling given by $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$, where U_4 refers to infinite edge coupling.

Let k_0 satisfying $\det\left[(1-k_0)U_4 - (1+k_0)I\right] \neq 0$ be a pole of the resolvent $(H - \lambda\,\mathrm{id})^{-1}$ of a multiplicity d. Let Γ_ε be a geometrically perturbed quantum graph with edge lengths $l_i(1+\varepsilon)$ and the same coupling. Then there is $\varepsilon_0 > 0$ s.t. for all $\vec{\varepsilon} \in \mathcal{U}_{\varepsilon_0}(0)$ the sum of multiplicities of the resolvent poles in a sufficiently small neighbourhood of k_0 is d.

Remark: The result holds only perturbatively, for larger values of ε poles may, e.g., escape to infinity.

hird resonance problem: Weyl asymptotic

Let us now look into *high-energy asymptotics* of graph resonances. Introduce *counting function* $N(R, F)$ as the number of zeros of $F(k)$ in the circle $\{k : |k| < R\}$ of given radius $R > 0$, algebraic multiplicities taken into account.

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Let us look how the situation looks like for graphs with 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 secular eq-n 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

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

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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: 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 $\sigma_r \in \mathbb{R}$, $\sigma_0 < \sigma_1 < \ldots < \sigma_n$. Suppose that $\lim_{k\to\infty} a_0(k) \neq 0$ and $\lim_{k\to\infty} a_n(k) \neq 0$. There exist a compact $\Omega \subset \mathbb{C}$, real numbers m_r and positive K_r, $r = 1, \ldots, n$, 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 the theorem

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

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

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

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By a direct computation we get

Lemma: The coefficient of $e^{\pm}$ in the above equation is $\left(\frac{i}{2}\right)^N \det\left[(\tilde{U}(k)-I)\pm k(\tilde{U}(k)+I)\right]$

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 $W < V$ (graph is non-Weyl in the terminology of [Davies-Pushnitski'10] 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 entries equal to one.

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

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

Unbalanced non-Weyl graphs

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

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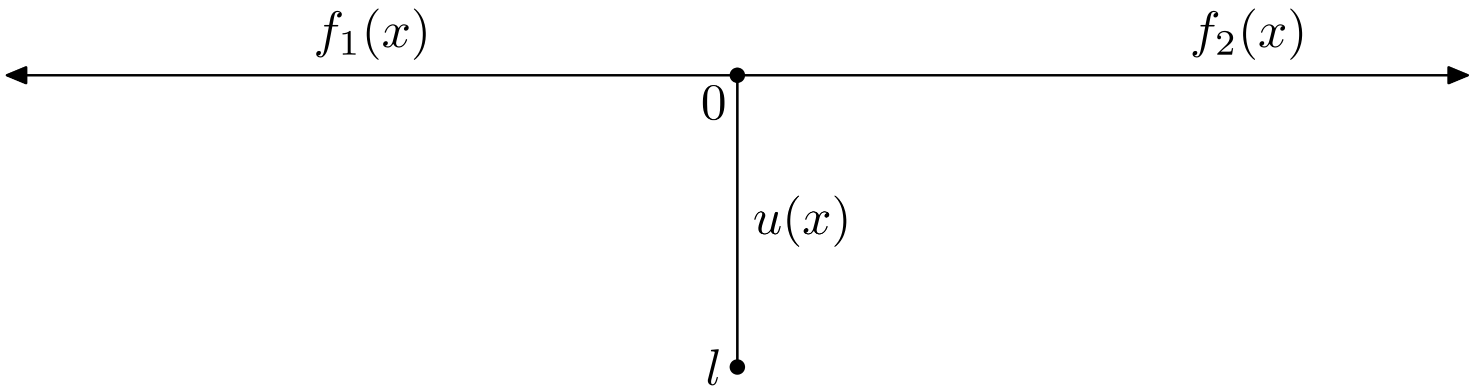
One can check easily the following claim

Lemma: 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

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

$f_i(x)$ 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

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

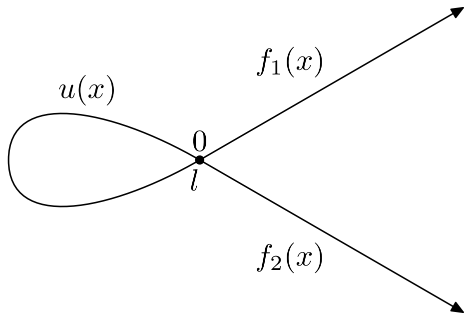
Remark

In particular, for Dirichlet condition both at the end of the separated half-line, $\psi = \pi$, and at the remote end of the internal edge, $c = 0$, one obtains a family of Hamiltonians which have no resonances at all. This includes $\varphi_1 = \varphi_2 = 0$ and $r = 1/\sqrt{2}$, or the conditions

$$f_1(0) = f_2(0), \quad u(0) = \sqrt{2} f_1(0), \quad f_1'(0) - f_2'(0) = -\sqrt{2} u'(0) \,,$$

where the fact of resonance absence was first noted in [E-Šerešová'94], and a similar behavior for $\varphi_1 = \varphi_2 = \pi$ and $r = 1/\sqrt{2}$. Notice that the absence of resonances is easily understood if one regards the graph in question as a tree and employs a unitary equivalence proposed first by Solomyak – see, e.g., [Sobolev-Solomyak'02].

Example: a loop with two leads



To illustrate how the asymptotics can *change with the graph geometry*, consider the above graph. The Hamiltonian acts as above with coupling conditions

$$\begin{aligned} u(0) = f_1(0)\,, \quad u(l) = f_2(0)\,, \\ \alpha u(0) = u'(0) + f_1'(0) + \beta(-u'(l) + f_2'(0))\,, \\ \alpha u(l) = \beta(u'(0) + f_1'(0)) - u'(l) + f_2'(0) \end{aligned}$$

with real parameters $\alpha,\,\beta \in \mathbb{R}$. The choice $\beta = 1$ gives the "overall" δ-condition of strength α, while $\beta = 0$ corresponds to a line with two δ-interactions at the distance l.

Example, continued

Using $\mathrm{e}_\pm = \mathrm{e}^{\pm ikx}$ we write the resonance condition as

$$8\frac{i\alpha^2 \mathrm{e}_+ + 4k\alpha\beta - i[\alpha(\alpha - 4ik) + 4k^2(\beta^2 - 1)]\, \mathrm{e}_-}{4(\beta^2 - 1) + \alpha(\alpha - 4i)} = 0\,.$$

The coefficient of e^+ vanishes *iff* $\alpha = 0$, the second term vanishes for $\beta = 0$ or if $|\beta| \neq 1$ and $\alpha = 0$, while the polynomial multiplying e^- does not vanish for any combination of α and β.

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In other words, the graph has a *non-Weyl asymptotics* *iff* $\alpha=0$. If, in addition, $|\beta|\neq 1$, than all resonances are confined to some circle, i.e. the graph "size" is zero. The exceptions are Kirchhoff condition, $\beta=1$ and $\alpha=0$, and its counterpart, $\beta=-1$ and $\alpha=0$, for which "one half" of the resonances is preserved, the "size" being $l/2$.

Example, continued

Let us look at the δ-condition, $\beta = 1$, to illustrate the disappearance of half of the resonances when the coupling strength vanishes. The resonance equation becomes

$$\frac{-\alpha \sin kl + 2k(1 + i \sin kl - \cos kl)}{\alpha - 4i} = 0$$

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A simple calculation shows that there is a sequence of embedded ev's, $k = 2n\pi/l$ with $n \in \mathbb{Z}$, and a family of resonances given by solutions to $\mathrm{e}^{ikl} = -1 + \frac{4ik}{\alpha}$. The former do not depend on α, while the latter behave for small α as

$$\operatorname{Im} k = -\frac{1}{l} \log \frac{1}{\alpha} + \mathcal{O}(1)\,, \quad \operatorname{Re} k = n\pi + \mathcal{O}(\alpha)\,,$$

thus all the (true) resonances escape to infinity as $\alpha \to 0$.

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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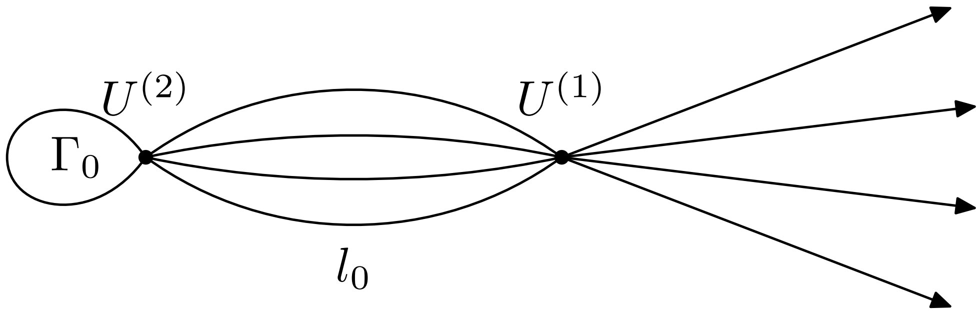

Consider the above graph with a balanced vertex $\mathcal{X}_1$ which connects p internal edges of the same length l_0 and p external edges with the coupling given by a unitary $U^{(1)} = aJ_{2p\times 2p} + bI_{2p\times 2p}$. The coupling to the rest of the graph, denoted as Γ_0, is described by a $q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

Unitary equivalence again

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

Application to symmetric coupling

Let now $U^{(1)} = aJ_{2p\times 2p} + bI_{2p\times 2p}$ 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 $\frac{1}{\sqrt{p}}(1, 1, \dots, 1)^{\mathrm{T}}$. The transformed matrix $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ decouples into blocks connecting only pairs (v_j, g_j).

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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*.

Effective size is a global property

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

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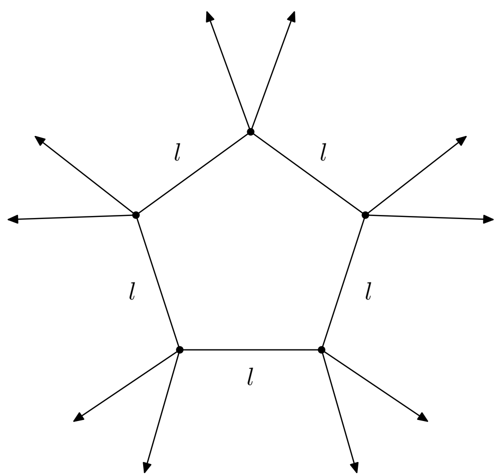

For a fixed integer $n \geq 3$ we start with a regular n-gon, each edge having length ℓ, and attach two semi-infinite leads to each vertex, so that each vertex is balanced; thus the *effective size W_n is strictly less than $V_n = n\ell$*.

Example, continued

Proposition: The effective size of the graph Γ_n is given by

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

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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 $n = 0 \mod 4$. $\square$

Concluding remarks

The present results inspire various questions, e.g.

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- Effect of *more general geometric perturbations*, possibly in combination with *external fields* on quantum graph spectra and resonances
- Can the inequality for resonances be valid *not only asymptotically*, in the spirit of Pólya conjecture for Dirichlet Laplacians?
- How these effects will look like for *more general operators*? in [DEL'10] criteria for occurrence of non-Weyl asymptotics were derived for weighted Laplacians, but there are others

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The present results inspire various questions, e.g.

- Effect of *more general geometric perturbations*, possibly in combination with *external fields* on quantum graph spectra and resonances
- Can the inequality for resonances be valid *not only asymptotically*, in the spirit of Pólya conjecture for Dirichlet Laplacians?
- How these effects will look like for *more general operators*? in [DEL'10] criteria for occurrence of non-Weyl asymptotics were derived for weighted Laplacians, but there are others
- etc.

The results discussed here come from

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[DP10] E.B. Davies, A. Pushnitski: Non-Weyl resonance asymptotics for quantum graphs, `arXiv: 1003.0051 [math.SP]`

[DEL10] E.B. Davies, P.E., J. Lipovský: NNon-Weyl asymptotics for quantum graphs with general coupling conditions, *J. Phys. A: Math. Theor.* **A43** (2010), to appear; `arXiv: 1004.08560 [math-phys]`

[DET08] P. Duclos, P.E., O. Turek: On the spectrum of a bent chain graph, *J. Phys. A: Math. Theor.* **A41** (2008), 415206

[EL10] P.E., J. Lipovský: Resonances from perturbations of quantum graphs with rationally related edges, *J. Phys. A: Math. Theor.* **A43** (2010), 105301

Thank you for your attention!