Quantum Graphs
and their generalizations

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Lecture III

Geometric perturbations of quantum graphs and properties of resonances

Lecture overview

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- note that these are just a few of many claims one can make about spectral and scattering properties of quantum graphs

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Geometric perturbations

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
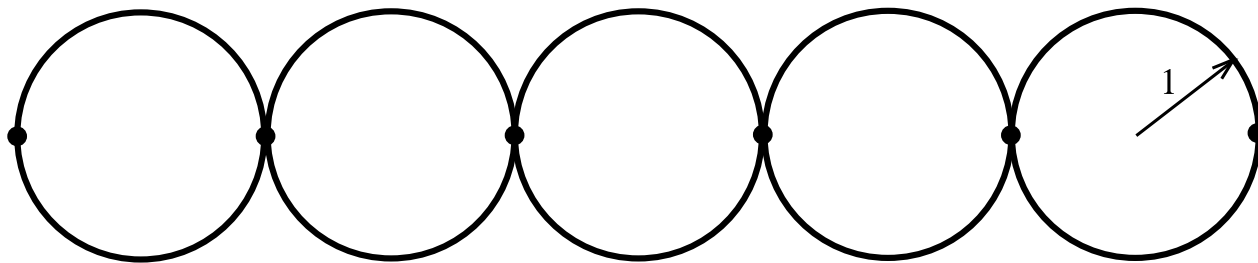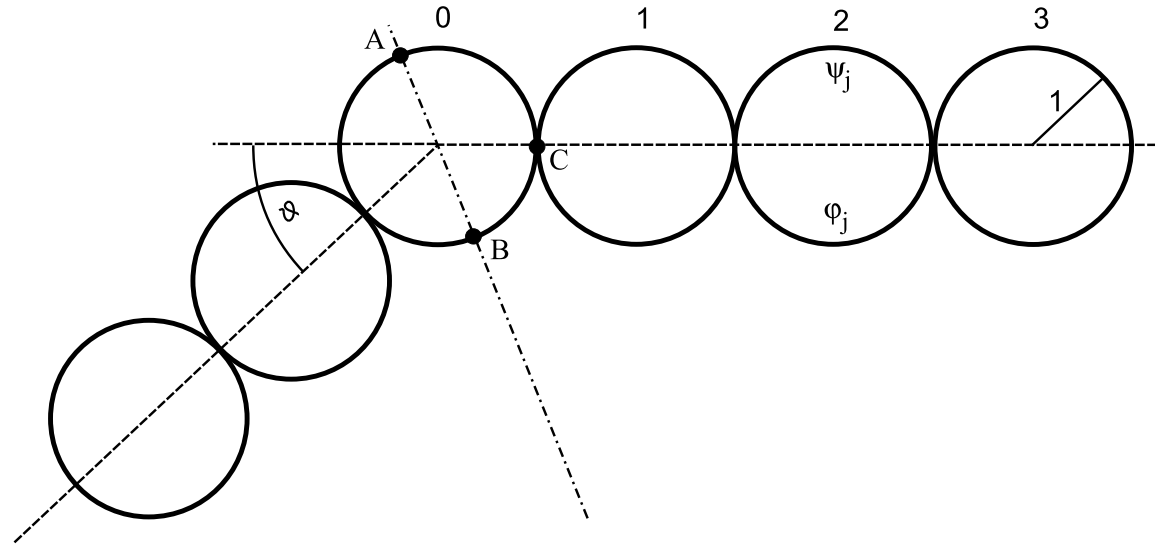

Without loss of generality we assume unit radii; the rings are connected by the δ-*coupling* of a strength $\alpha \neq 0$
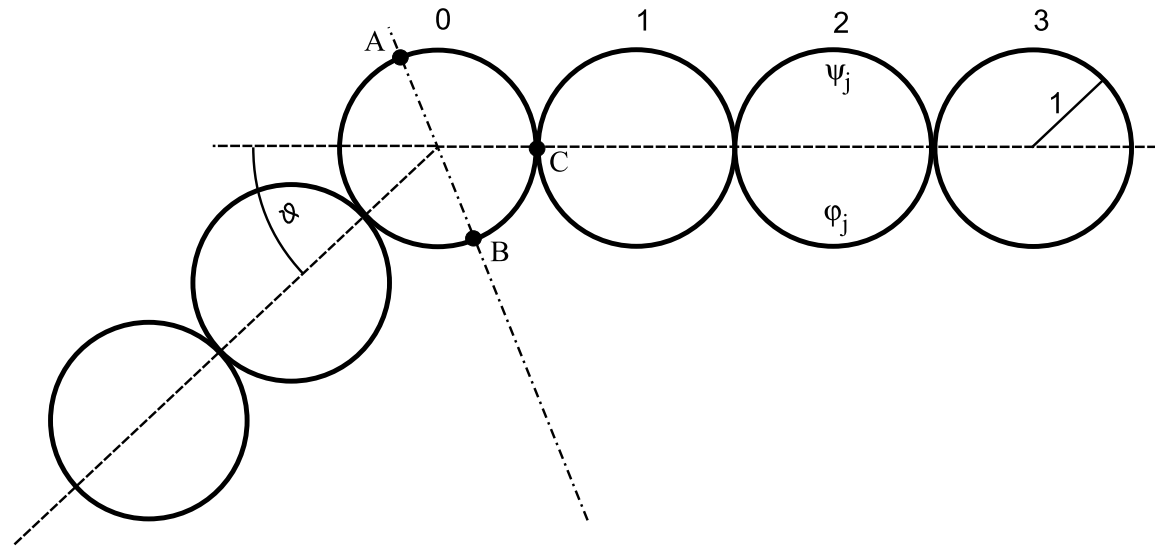
Bending the chain

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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

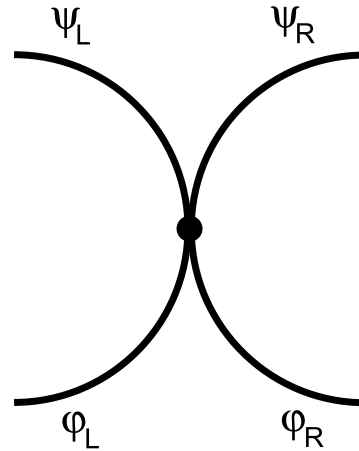- the bent chain exhibits also *resonances*

An infinite periodic chain

The "straight" chain Γ_0 can be treated as a periodic system analyzing the spectrum of the elementary cell
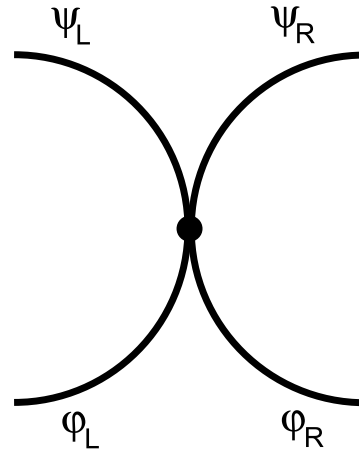
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This yields the condition

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

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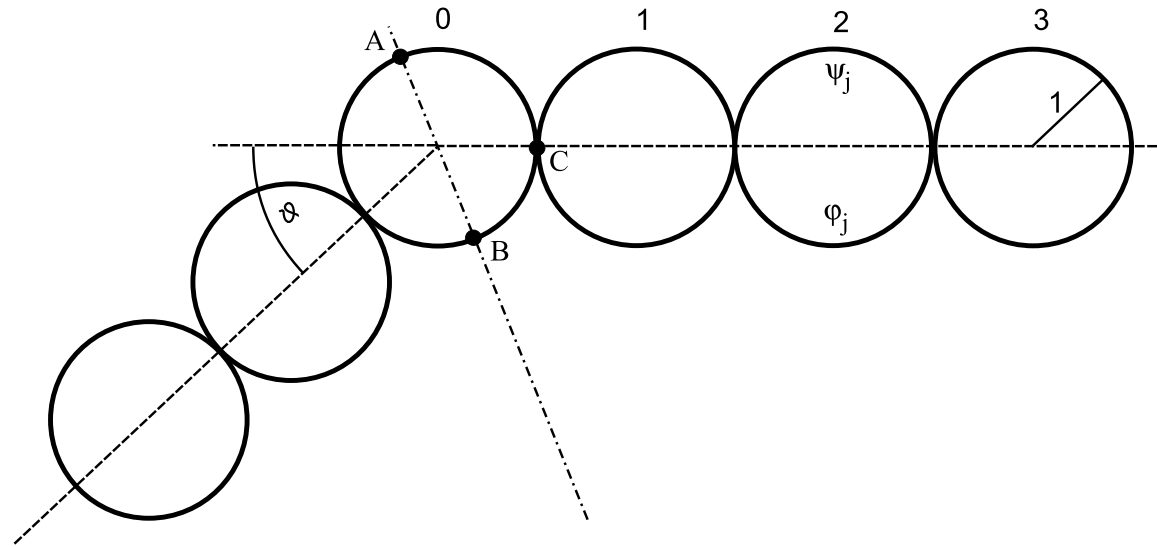Finally, $\sigma(H_0) = [0, +\infty)$ holds if $\alpha = 0$.

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*

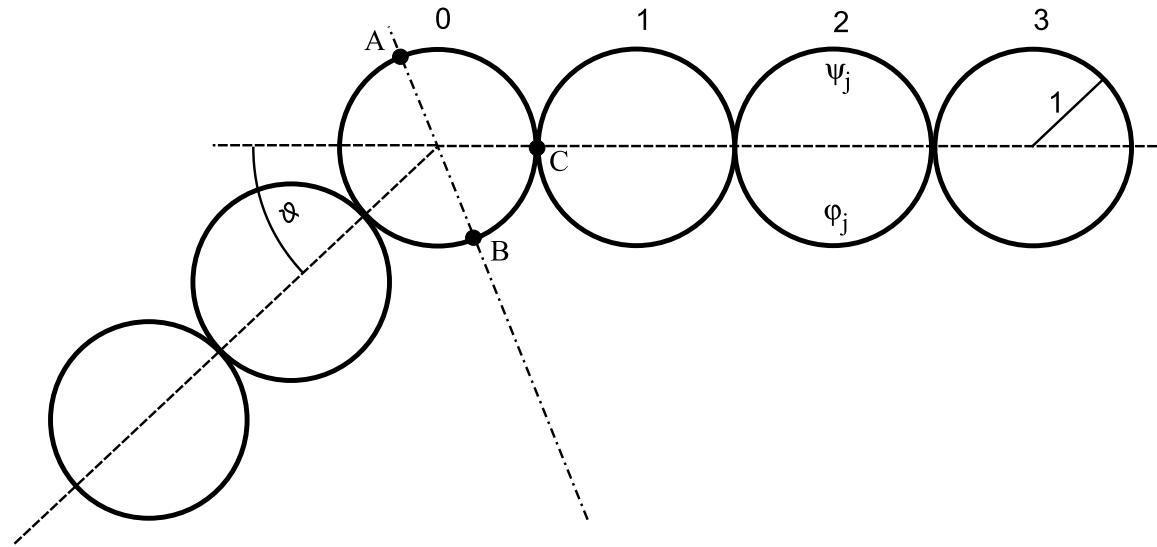- It is also an example of *gaps coming from decoration*

The bent chain spectrum

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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 $\mathrm{e}^{\pm\text{ß}kx}$,

$$
\begin{aligned}
\psi_j(x) &= C_j^+ \mathrm{e}^{\text{ß}kx} + C_j^- \mathrm{e}^{-\text{ß}kx}, \quad x \in [0, \pi], \\
\varphi_j(x) &= D_j^+ \mathrm{e}^{\text{ß}kx} + D_j^- \mathrm{e}^{-\text{ß}kx}, \quad x \in [0, \pi]
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for $j \in \mathbb{N}$. On the other hand, for $j = 0$ we have

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\psi_0(x) &= C_0^+ \mathrm{e}^{\text{ß}kx} + C_0^- \mathrm{e}^{-\text{ß}kx}, \quad x \in \left[\frac{\pi - \vartheta}{2}, \pi\right] \\
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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 $j \geq 2$

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

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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*

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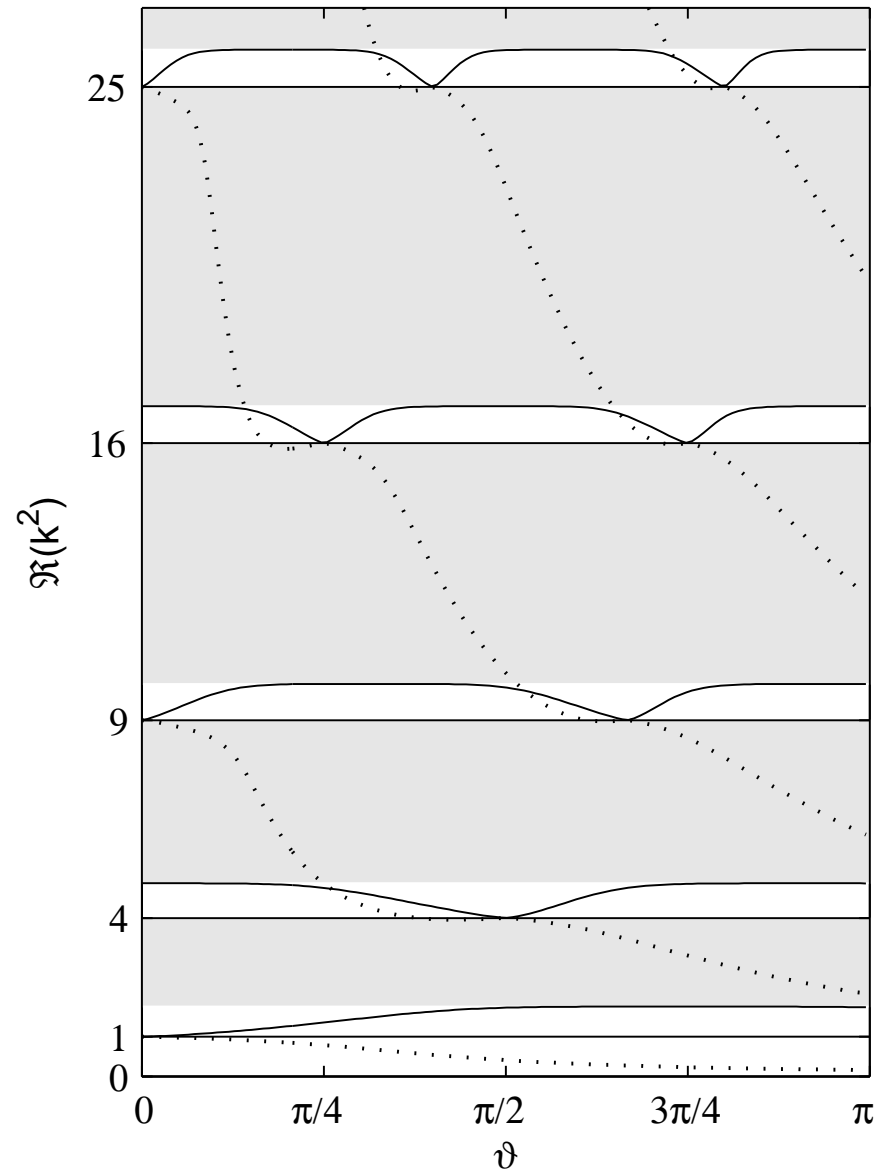
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After a tiresome but straightforward analysis one arrives then at the following conclusion:

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 $\alpha = 3$

Spectrum of H^-

Replacing Neumann condition by Dirichlet at the mirror axis we get the spectral condition in this case,

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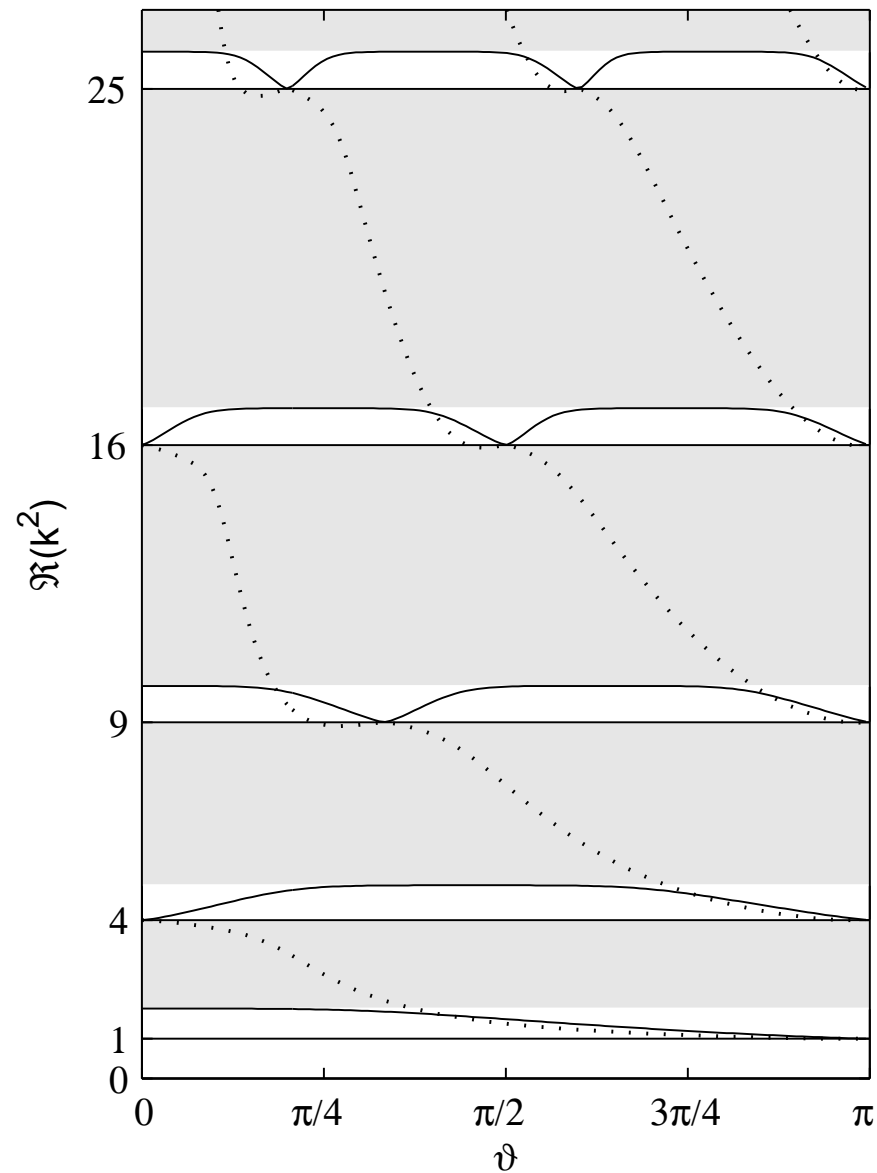$$-\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}$$

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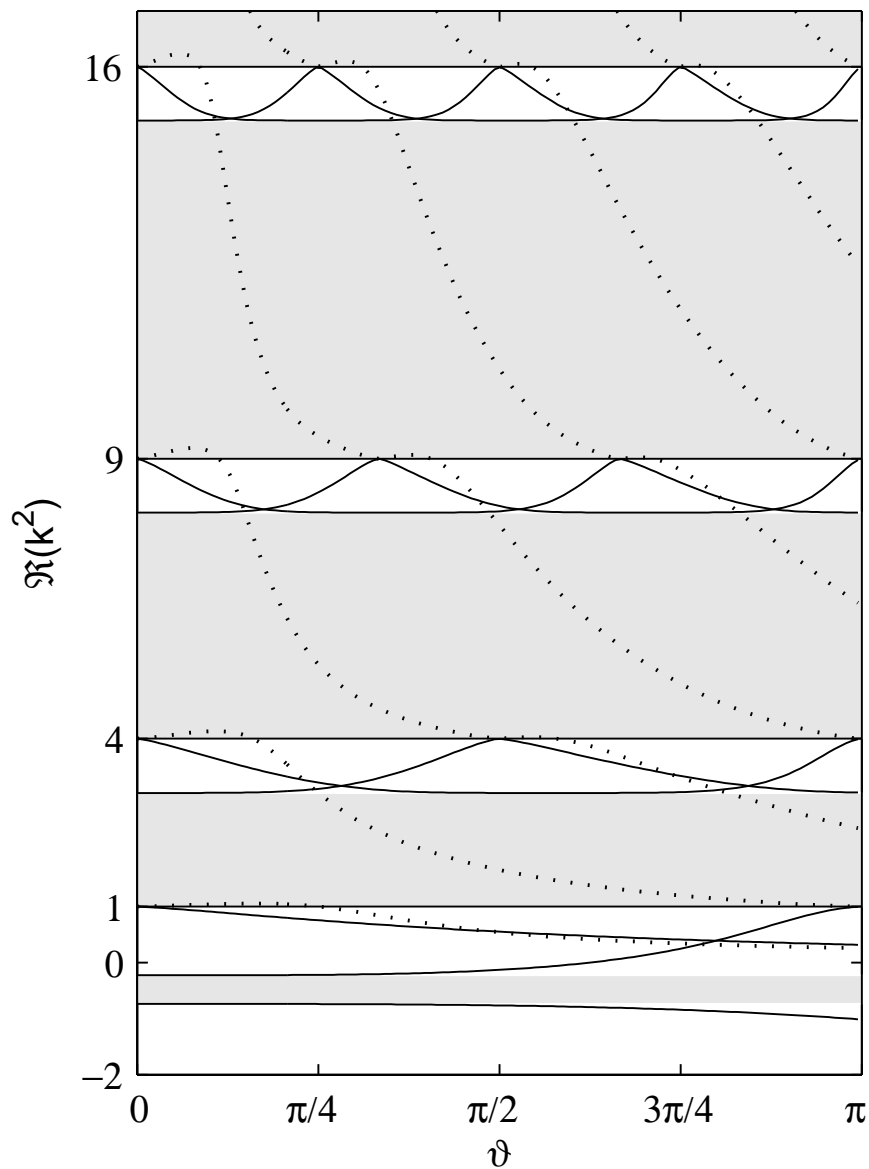
$$k \cdot \tan k\pi = \frac{\alpha}{2}$$

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

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

Resonances, analyticity

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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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, $\alpha = 3$
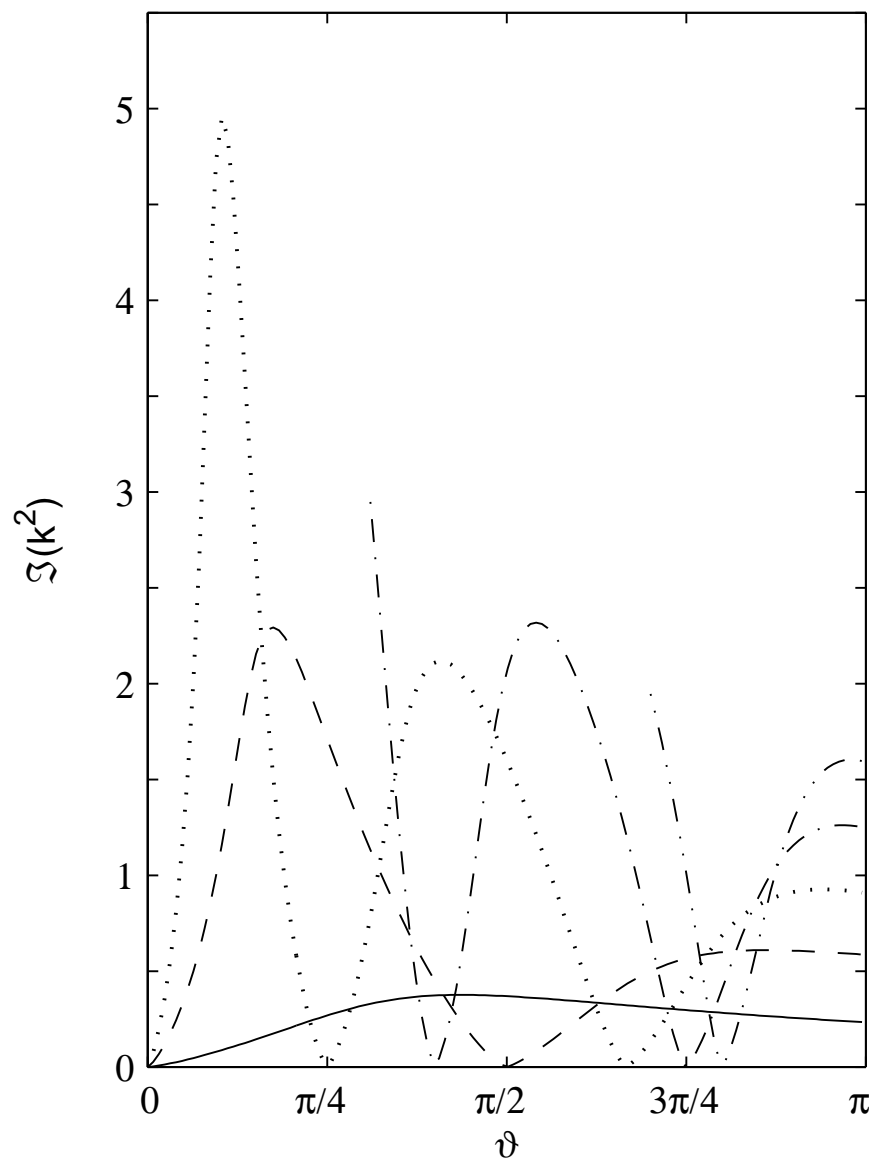
More on the angle dependence

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

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

so he curve is indeed non-analytic there. The same is true for $\vartheta_0 = 0$ provided the band-edge value k_0 is odd

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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

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

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: The fourth-power is the same as for the ground state of a *slightly bent Dirichlet tube* [Duclos-E'95] despite the fact that the dynamics is very different in the two cases

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Remark: The analogous problem for *bent leaky wires* studied in [E-Ichinose'01] remains open – see Lecture IV

Another problem concerning resonances

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- Most typical resonance situations arise for *finite graphs with semiinfinite leads*

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- *Different resonances definitions:* poles of continued resolvent, singularities of on-shell S matrix

- Graphs may exhibit embedded eigenvalues due to *invalidity of uniform continuation*

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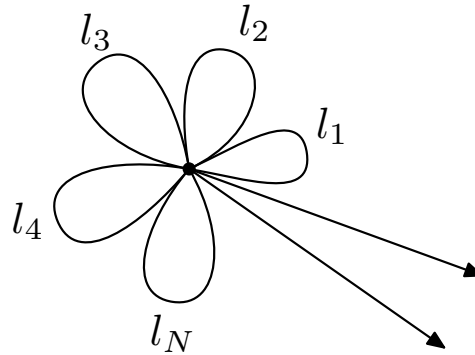The Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$ on each link satisfying the boundary conditions

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

characterized by unitary matrices U_j at the vertices $\mathcal{X}_j$.
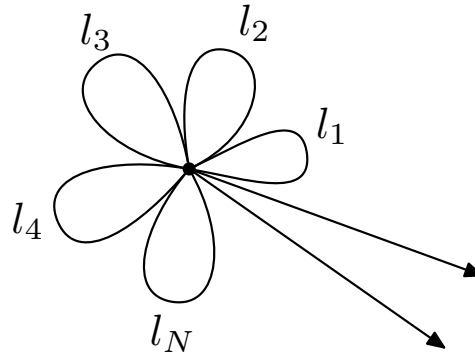
A universal setting for graphs with leads

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

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

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

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 resonance definitions

Resonances as poles of analytically continued resolvent,
$(H - \lambda \operatorname{id})^{-1}$. 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

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

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

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

$$\det\,[(U - I)\,C_1(k) + ik(U + I)\,C_2(k)] = 0$$

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$$\det \left[(U - I) \, C_1(k) + ik(U + I) \, C_2(k) \right] = 0$$

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

$$(\tilde{U}(k) - I)(f_1, \ldots, f_{2N})^{\mathrm{T}} + i(\tilde{U}(k) + I)(f_1', \ldots, f_{2N}')^{\mathrm{T}} = 0,$$
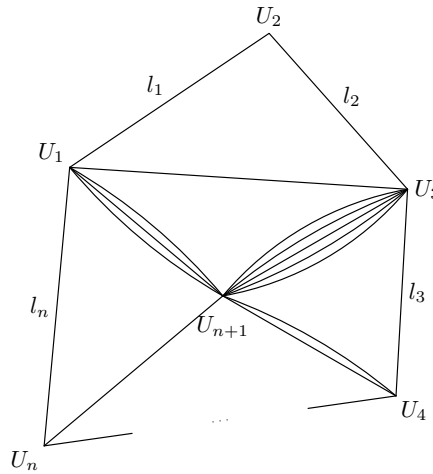
where the corresponding coupling matrix

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

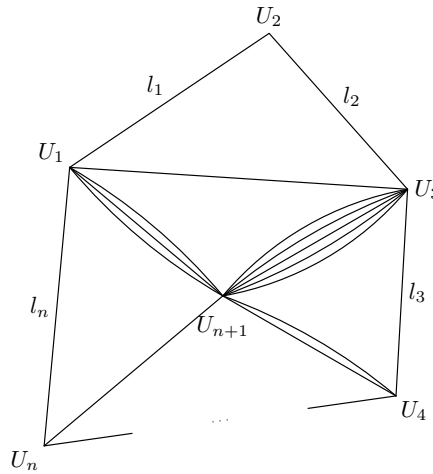is obviously *energy-dependent* and, in general, *non-unitary*

Embedded ev's for commensurate edges

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

Embedded ev's for commensurate edges

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

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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\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}
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Example: a loop with two leads
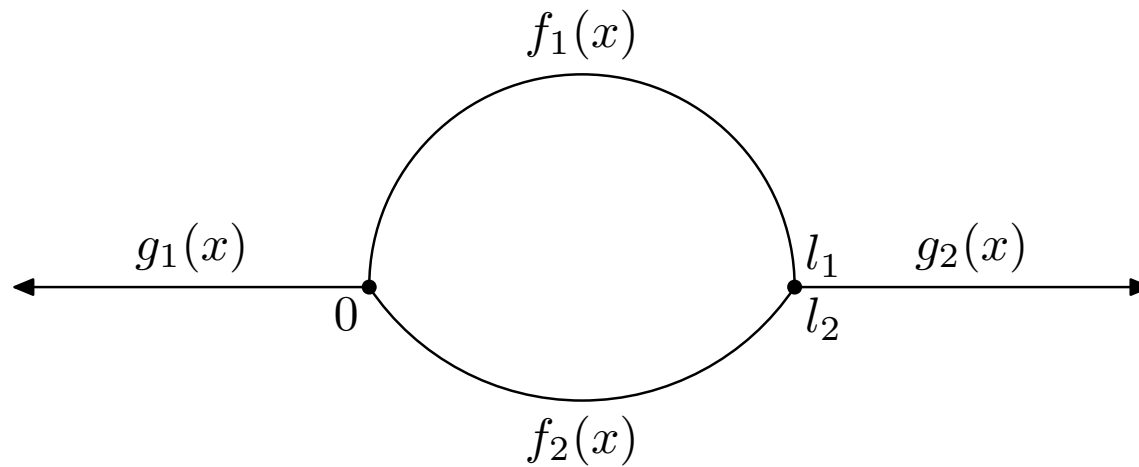
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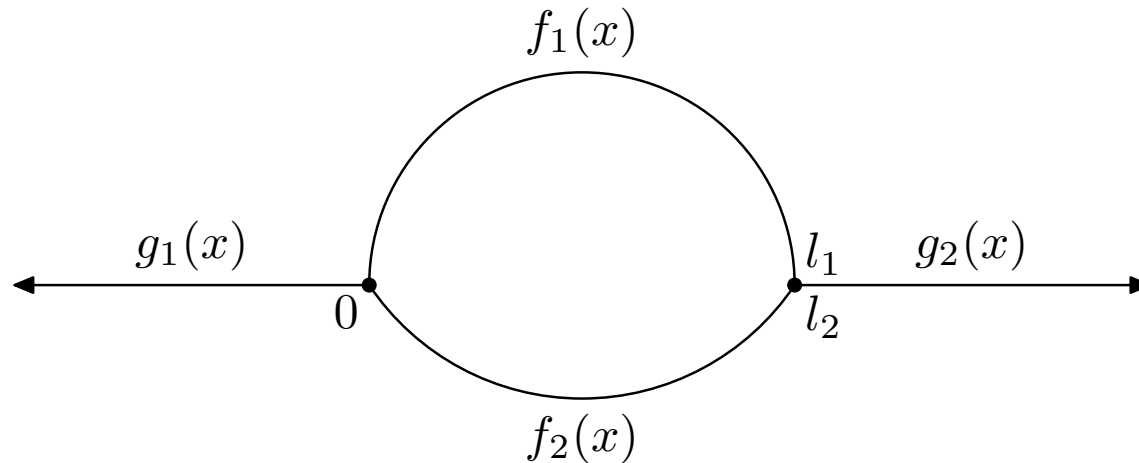
The setting is as above, the b.c. at the nodes are

$$
\begin{aligned}
f_1(0) &= f_2(0), \qquad f_1(l_1) = f_2(l_2), \\
f_1(0) &= \alpha_1^{-1}(f_1'(0) + f_2'(0)) + \gamma_1 g_1'(0), \\
f_1(l_1) &= -\alpha_2^{-1}(f_1'(l_1) + f_2'(l_2)) + \gamma_2 g_2'(0), \\
g_1(0) &= \bar{\gamma}_1(f_1'(0) + f_2'(0)) + \tilde{\alpha}_1^{-1} g_1'(0), \\
g_2(0) &= -\bar{\gamma}_2(f_1'(l_1) + f_2'(l_2)) + \tilde{\alpha}_2^{-1} g_2'(0)
\end{aligned}
$$

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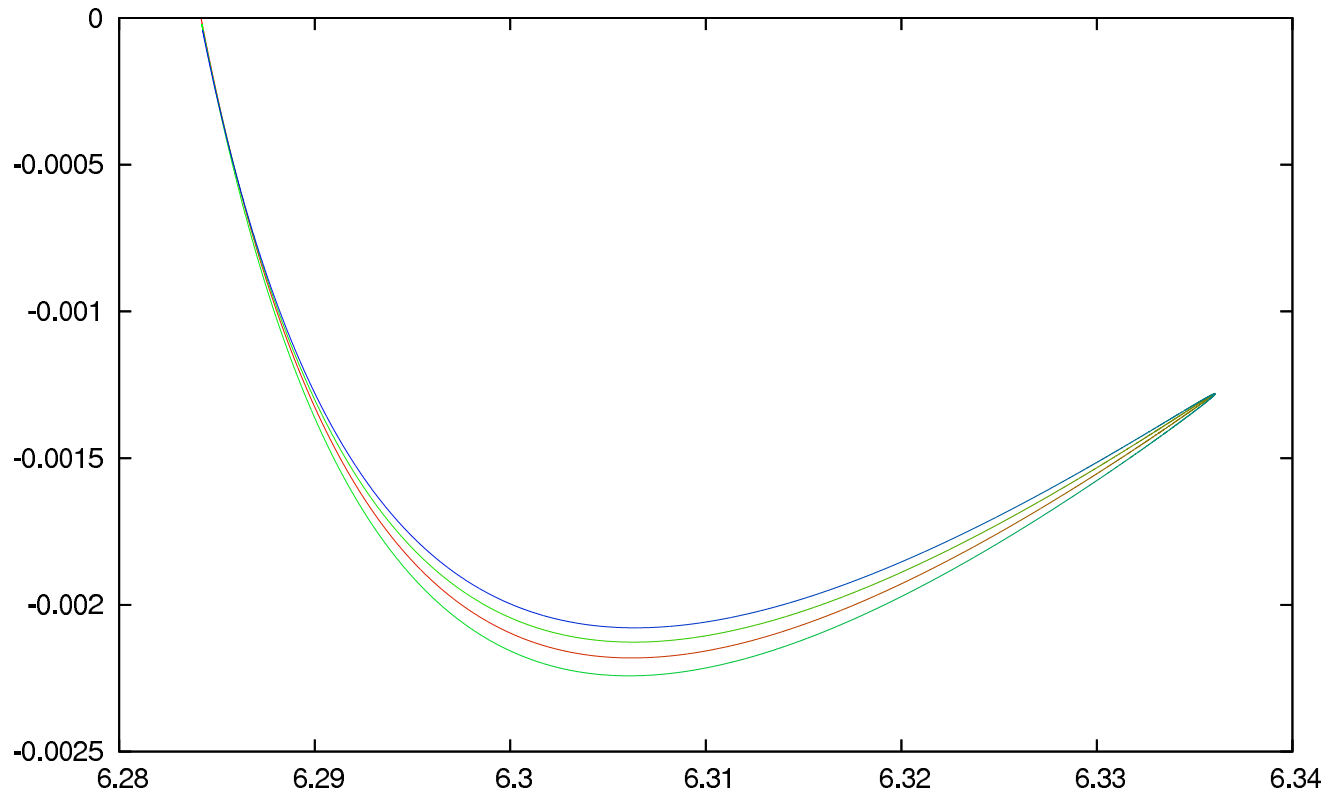
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The condition can be solved numerically to find the resonance trajectories with respect to the variable λ.
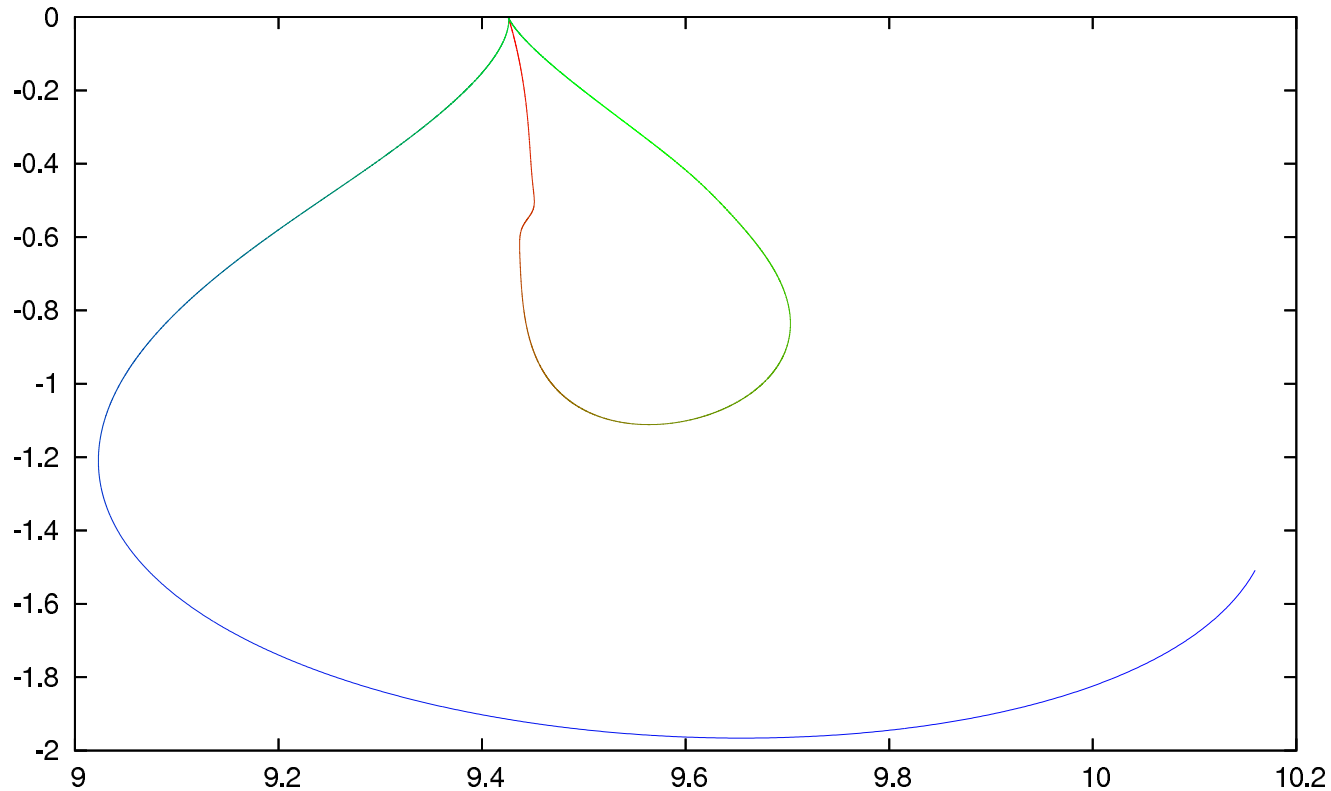
Pole trajectory

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.
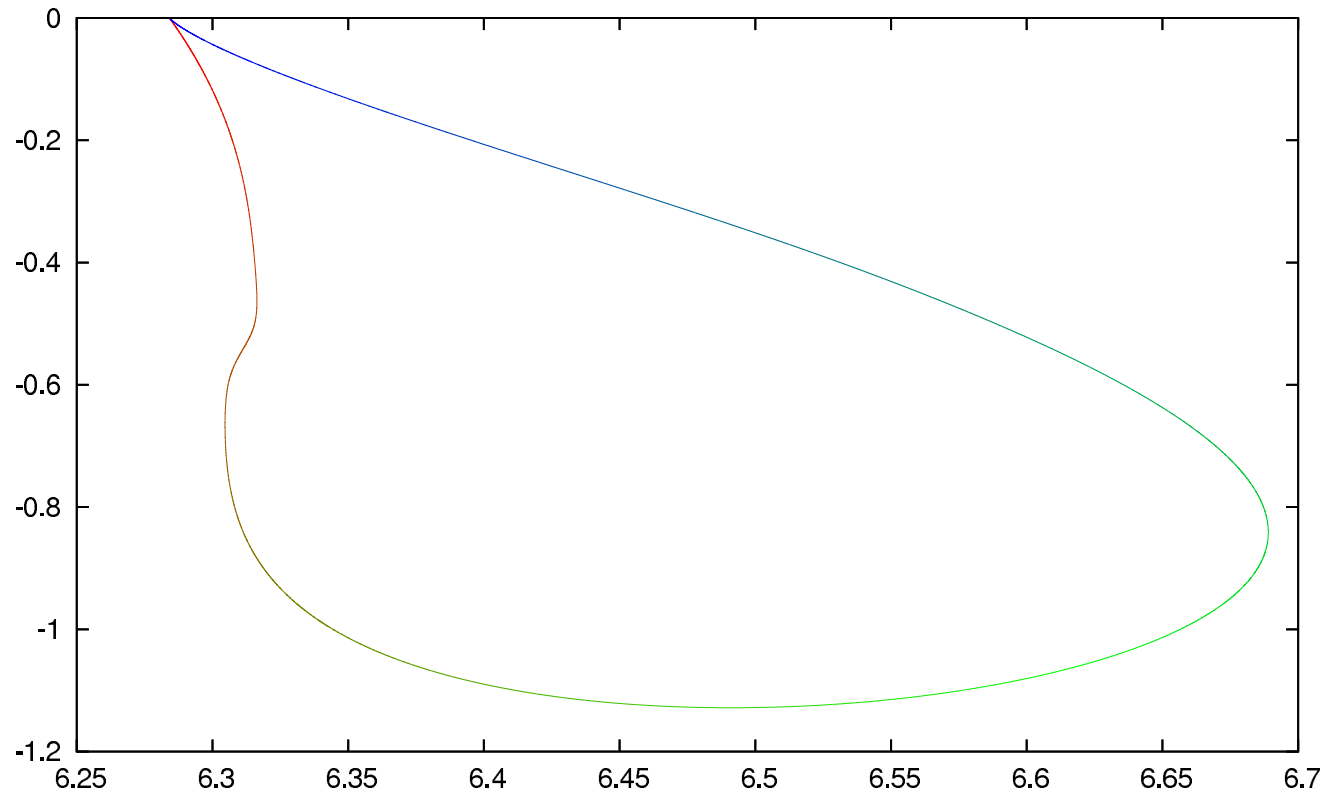
Pole trajectory

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

$$g_1(x) \qquad \begin{array}{c} f_1(x) \mid l_1 = l\,(1-\lambda) \\ \\ 0 \\ \\ f_2(x) \mid l_2 = l\,(1+\lambda) \end{array} \qquad g_2(x)$$

Example: a cross-shaped graph

$$f_1(x) \;\big|\; l_1 = l\,(1-\lambda)$$

$$g_1(x) \qquad\qquad\qquad\qquad g_2(x)$$

$$0$$

$$f_2(x) \;\big|\; l_2 = l\,(1+\lambda)$$
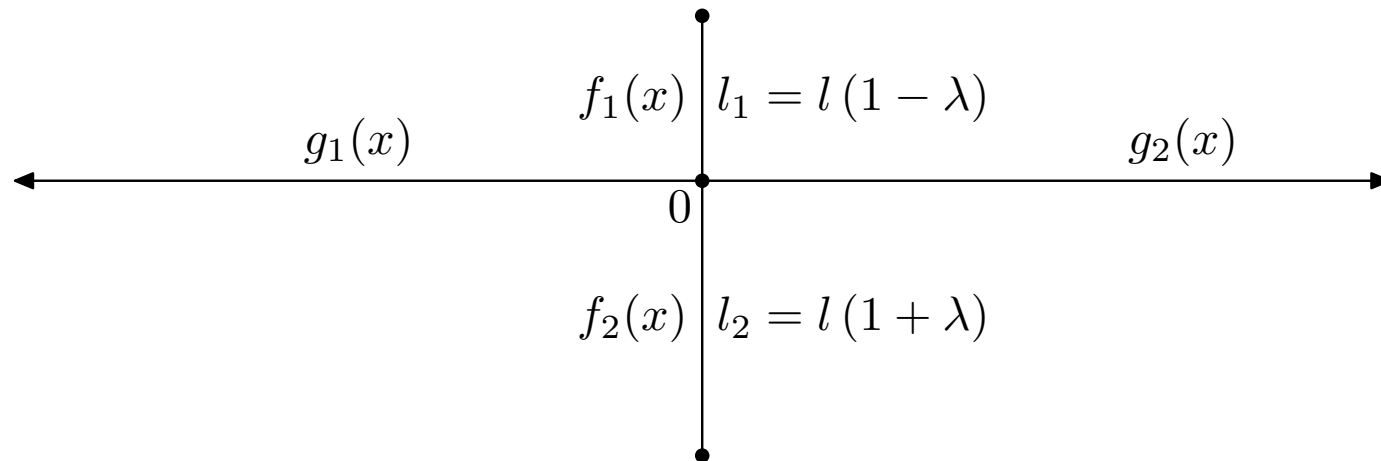
This time we restrict ourselves to the δ coupling as the boundary condition at the vertex and we consider Dirichlet conditions at the loose ends, i.e.

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

leading to the resonance condition
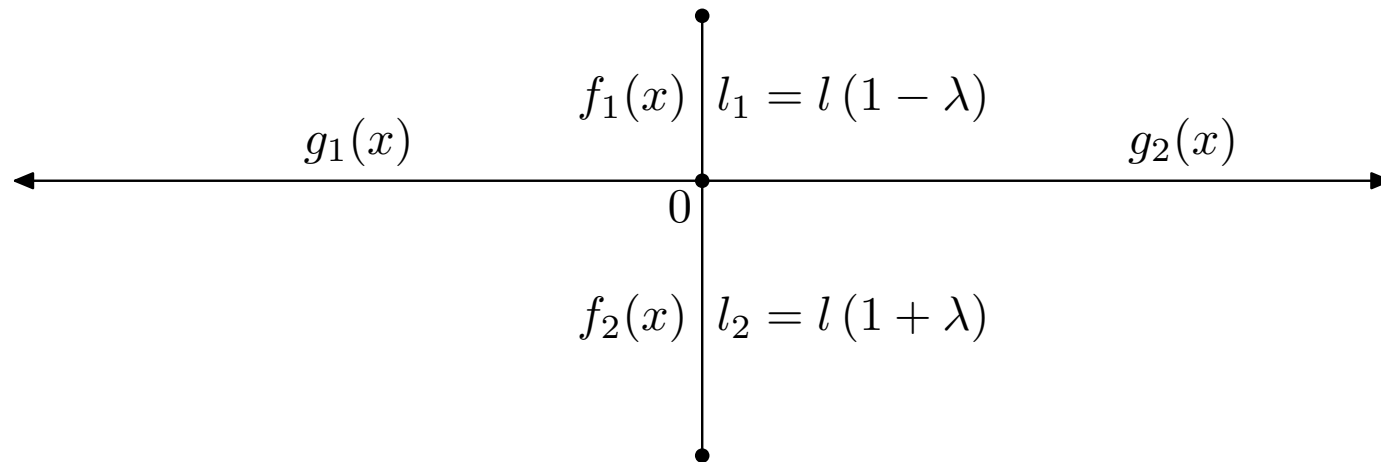
$$2k \sin 2kl + (\alpha - 2ik)(\cos 2kl\lambda - \cos 2kl) = 0$$

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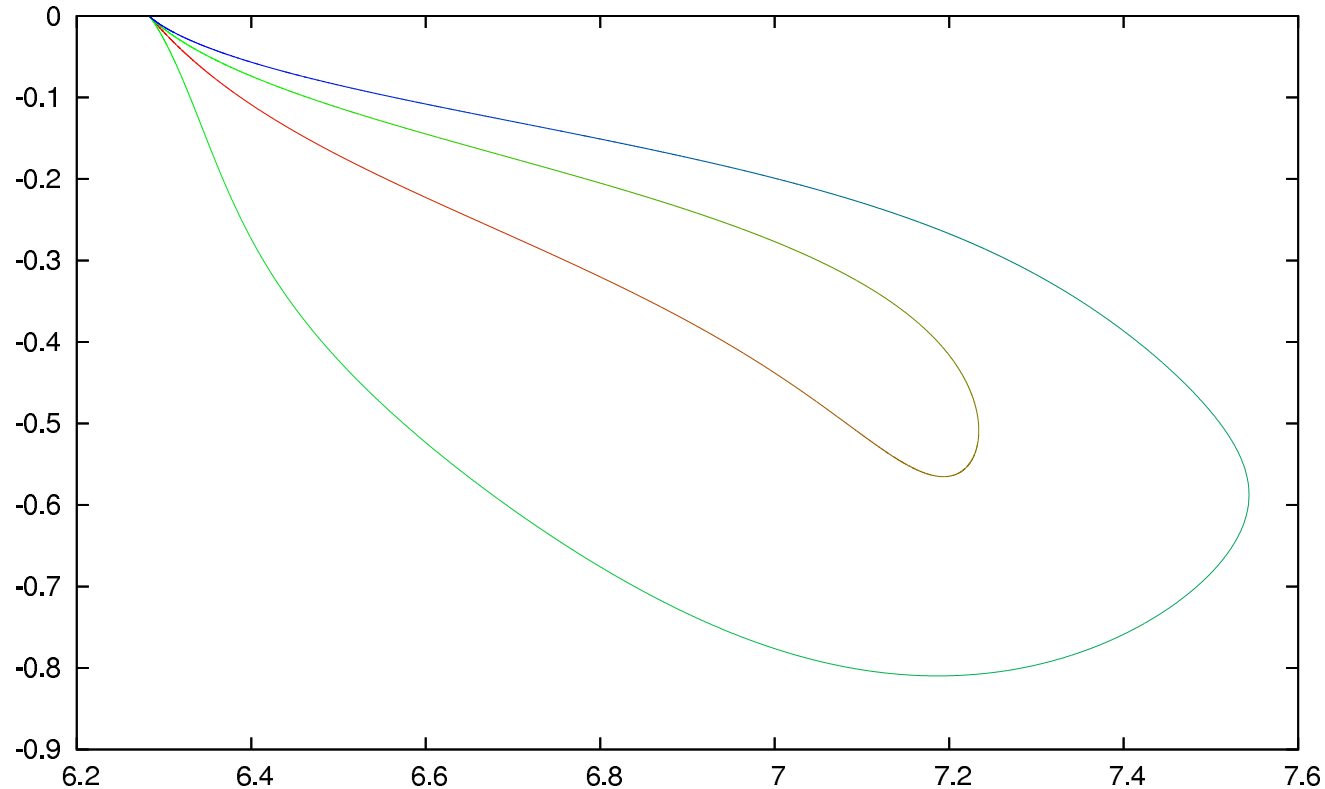
The trajectory of the resonance pole starting at $k_0 = 2\pi$ for the coefficients values $\alpha = 10$, $n = 2$. The colour coding is the same as in the previous figures.

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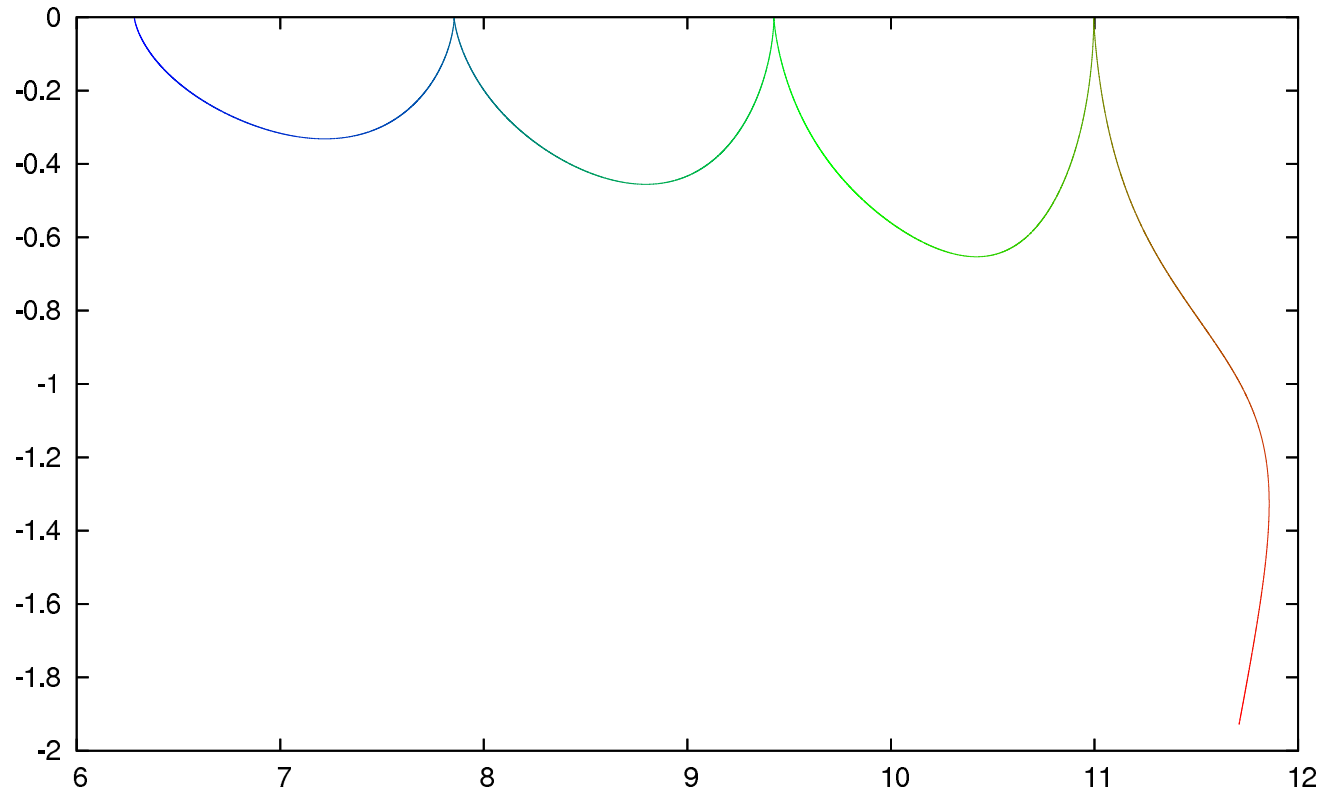
The trajectory of the resonance pole for the coefficients values $\alpha = 1$, $n = 2$. The colour coding is the same as above.

Pole trajectory
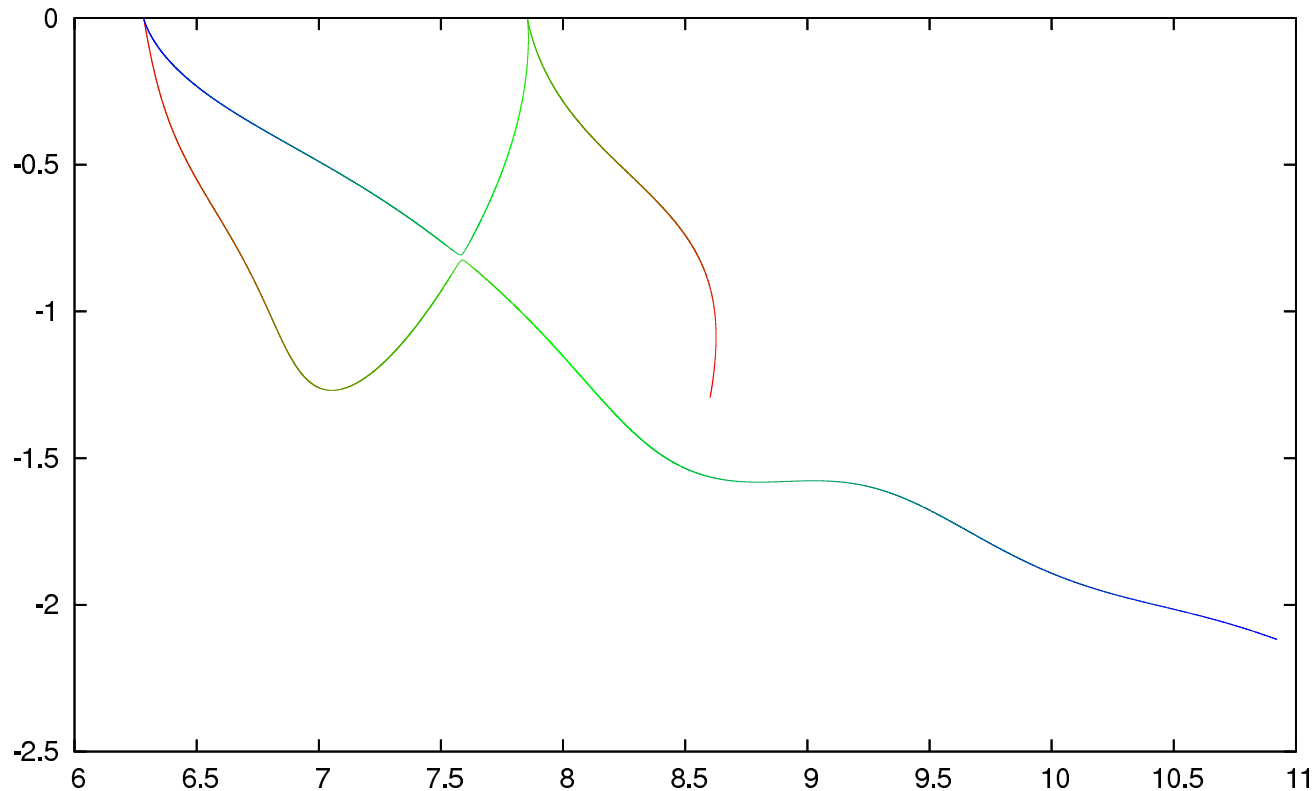
The trajectories of two resonance poles for the coefficients values $\alpha = 2.596$, $n = 2$. We can see an avoided resonance crossing – the former eigenvalue "travelling from the left to the right" interchanges with the former resonance "travelling the other way" and ending up as an embedded eigenvalue. 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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Remark: The result holds only perturbatively, for larger values of ε poles may, e.g., escape to infinity.

And another resonance problem

The paper [DET'08] also inspired [Davies-Pushnitski'10] 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.

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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

$$0 = \det \left\{ \frac{1}{2}[(U-I) + k(U+I)]E_1(k) + \frac{1}{2}[(U-I) + k(U+I)]E_2 + k(U+I)E_3 \right.$$

$$\left. + (U-I)E_4 + [(U-I) - k(U+I)] \operatorname{diag}(0,\dots,0,I_{M\times M}) \right\},$$

where $E_i(k) = \operatorname{diag}\left(E_i^{(1)}, E_i^{(2)}, \dots, E_i^{(N)}, 0, \dots, 0\right)$,

$i = 1, 2, 3, 4$, consists of N nontrivial 2×2 blocks

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

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: 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 $-\operatorname{Im} k + m_r \log |k| = \pm K_r$ 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,

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

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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\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 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

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

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 $U = a J_{n \times n} + b I_{n \times n}$ 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 $U = a J_{(p+q) \times (p+q)} + b I_{(p+q) \times (p+q)}$. Then the energy-dependent effective matrix is

$$\tilde{U}(k) = \frac{ab(1-k) - a(1+k)}{(aq+b)(1-k) - (k+1)} J_{p \times p} + b I_{p \times p}\,.$$

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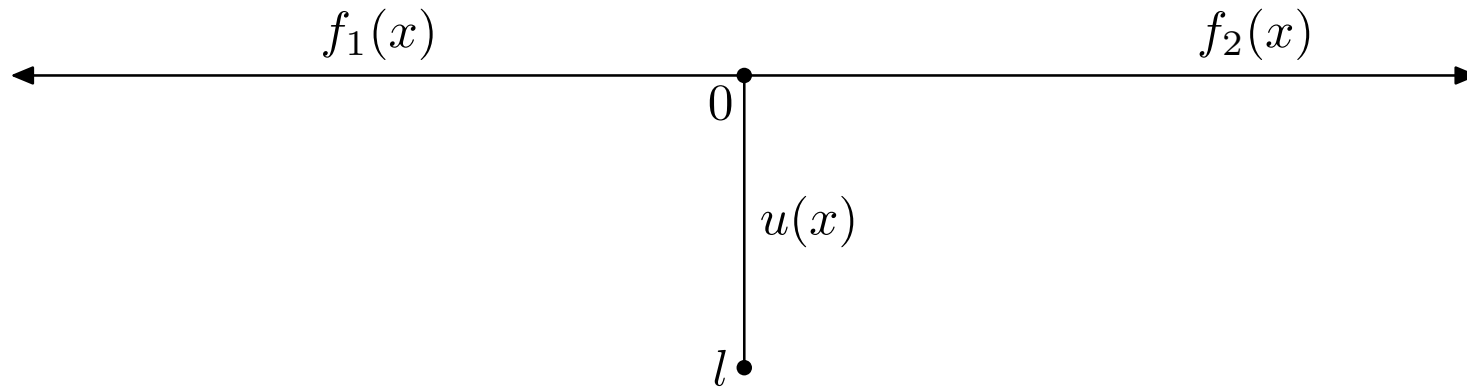
$$
W = \begin{pmatrix} \mathrm{e}^{i\varphi} I_{p \times p} & 0 \\ 0 & W_4 \end{pmatrix}
$$

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

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

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

Example, continued

We start from the matrix $U_0 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & e^{i\psi} \end{pmatrix}$, 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 $W = \begin{pmatrix} 1 & 0 & 0 \\ 0 & re^{i\varphi_1} & \sqrt{1-r^2}\,e^{i\varphi_2} \\ 0 & \sqrt{1-r^2}\,e^{i\varphi_3} & -re^{i(\varphi_2+\varphi_3-\varphi_1)} \end{pmatrix}$

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

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

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
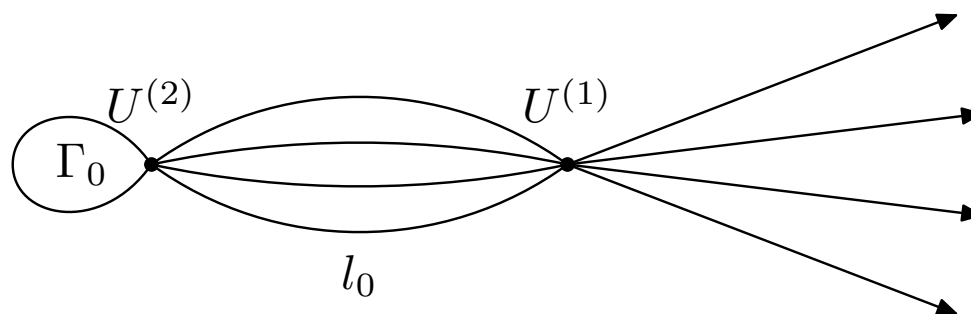
What can cause a non-Weyl asymptotics?

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

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, $V^{(1)} := \operatorname{diag}(V, V)$ and $V^{(2)} := \operatorname{diag}(I_{(q-p) \times (q-p)}, V)$ 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 $\frac{1}{\sqrt{p}}(1, 1, \ldots, 1)^{\mathrm{T}}$. 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 $j = 2, \ldots, p$.

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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:
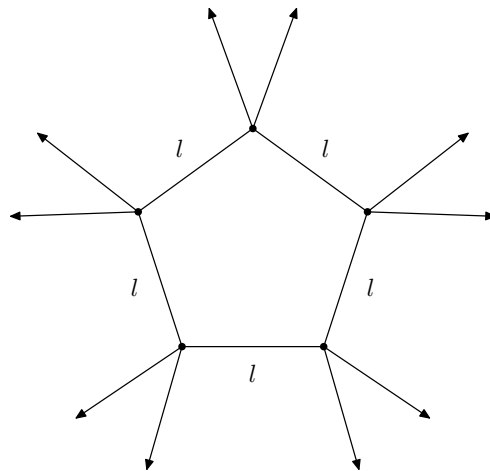
Effective size is a global property

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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

$$(U_j - I)\Psi_j + i(U_j + I)(\Psi_j' + i\mathcal{A}_j\Psi_j) = 0$$

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

Magnetic graph 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 $\begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}$ 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.

Proof: Using the effective coupling matrix $\tilde{U}(k)$ as in the non-magnetic case $\square$

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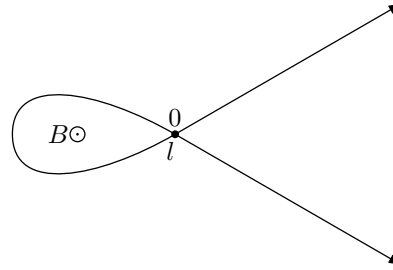
Proof: Using the effective coupling matrix $\tilde{U}(k)$ as in the non-magnetic case $\square$

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.
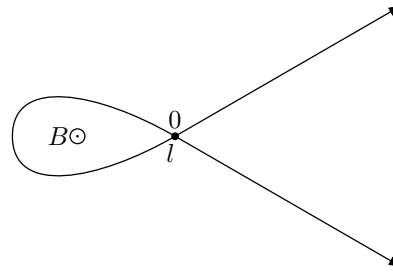
Example

The magnetic field can change, though, the effective size

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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 $\Phi = \pm\pi/2 \,(\mathrm{mod}\,\pi)$, 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*

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Summarizing Lecture III

- *Local geometric perturbations* of quantum graphs can produce eigenvalues in gaps as well as resonances

- *Embedded eigenvalues* of quantum graphs are generically unstable and can turn into resonances when the size ratios change

- *Resonances may not follow the Weyl law:* for particular graph topology and vertex coupling the effective size of the graph may be diminished

- A *magnetic field* cannot change a Weyl graph into a non-Weyl one but it can influence the size of non-Weyl graphs

Some literature to Lecture III

- [DEL10] E.B. Davies, P.E., J. Lipovský: Non-Weyl asymptotics for quantum graphs with general coupling conditions, *J. Phys. A: Math. Theor.* **A43** (2010), 474013

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

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

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

- [EL11] P.E., J. Lipovský: Non-Weyl resonance asymptotics for quantum graphs in a magnetic field, *Phys. Lett.* **A375** (2011), 805-807

Lecture IV

Leaky graphs – what they are, relations of their spectral and resonance properties

Lecture overview

- Why we might want *something better* than the ideal graph model of the previous lectures

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- Other type of *geometric perturbations*: making a hiatus on an edge

Drawbacks of ideal graphs

● Presence of *ad hoc parameters* in the b.c. describing branchings. A natural remedy: fit these using an approximation procedure, e.g.
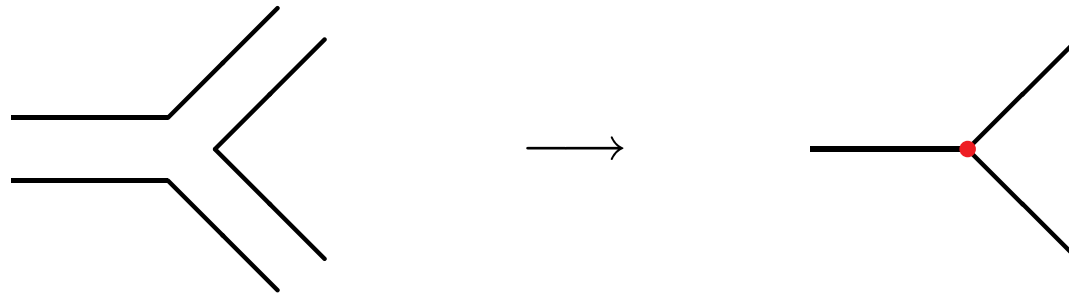
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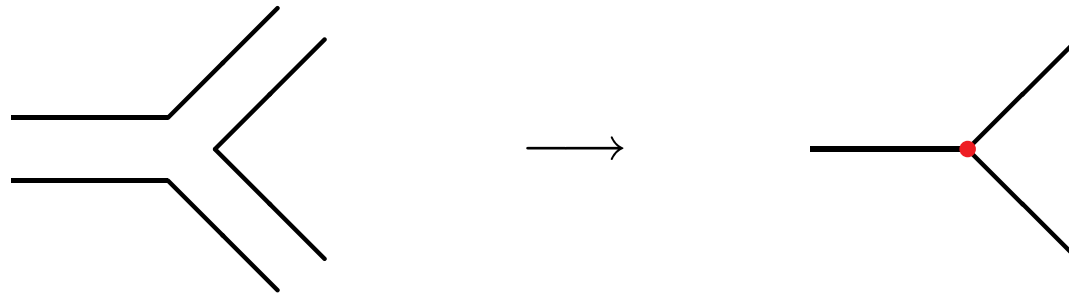
As we have seen in *Lectures I, II* it is possible but not exactly easy, and some work remains to be done

- More important, *quantum tunneling is neglected* in ideal graph models – recall that a true quantum-wire boundary is a *finite potential jump* – hence topology is taken into account but *geometric effects may not be*

Leaky quantum graphs

We consider *"leaky"* graphs with an *attractive interaction* supported by graph edges. Formally we have

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)\,, \quad \alpha > 0\,,$$

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A proper definition of $H_{\alpha,\Gamma}$: it can be associated naturally with the quadratic form,

$$\psi \mapsto \|\nabla\psi\|^2_{L^2(\mathbb{R}^n)} - \alpha \int_\Gamma |\psi(x)|^2 \mathrm{d}x\,,$$

which is closed and below bounded in $W^{2,1}(\mathbb{R}^n)$; the second term makes sense in view of Sobolev embedding. This definition also works for various "wilder" sets Γ

Leaky graph Hamiltonians

For Γ with locally finite number of smooth edges and *no cusps* we can use an *alternative definition* by boundary conditions: $H_{\alpha,\Gamma}$ acts as $-\Delta$ on functions from $W^{2,1}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \Gamma)$, which are continuous and exhibit a normal-derivative jump,

$$\frac{\partial\psi}{\partial n}(x)\Big|_{+} - \frac{\partial\psi}{\partial n}(x)\Big|_{-} = -\alpha\psi(x)$$

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$$\left. \frac{\partial\psi}{\partial n}(x) \right|_+ - \left. \frac{\partial\psi}{\partial n}(x) \right|_- = -\alpha\psi(x)$$

Remarks:

- *for graphs in $\mathbb{R}^3$* we use generalized b.c. which define a two-dimensional point interaction in normal plane

- one can combine *"edges" of different dimensions* as long as $\mathrm{codim}\,\Gamma$ does not exceed three
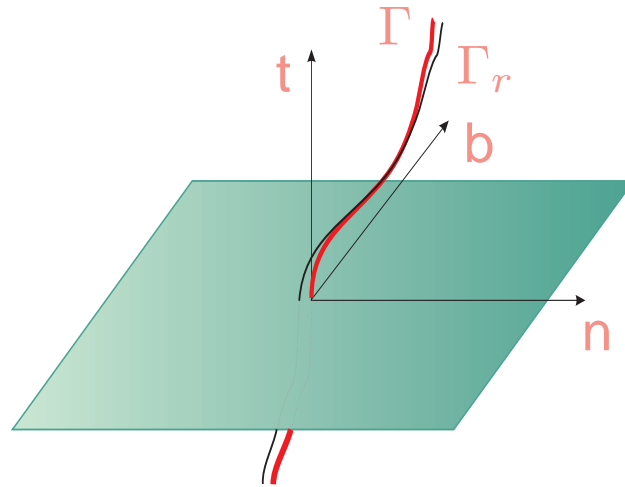
The case $\operatorname{codim} \Gamma = 2$

Boundary conditions can be used but they are more complicated. Moreover, for an infinite Γ corresponding to $\gamma : \mathbb{R} \to \mathbb{R}^3$ we have to assume in addition that there is a tubular neighbourhood of Γ which *does not intersect itself*

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Employ *Frenet's frame* $(t(s), b(s), n(s))$ for Γ. Given $\xi, \eta \in \mathbb{R}$ we set $r = (\xi^2 + \eta^2)^{1/2}$ and define family of "shifted" curves

$$\Gamma_r \equiv \Gamma_r^{\xi\eta} := \{\, \gamma_r(s) \equiv \gamma_r^{\xi\eta}(s) := \gamma(s) + \xi b(s) + \eta n(s) \,\}$$

The case $\operatorname{codim}\Gamma = 2$

The restriction of $f \in W_{\mathrm{loc}}^{2,2}(\mathbb{R}^3 \setminus \Gamma)$ to Γ_r is well defined for small r; we say that $f \in W_{\mathrm{loc}}^{2,2}(\mathbb{R}^3 \setminus \Gamma) \cap L^2(\mathbb{R}^3)$ belongs to Υ if

$$
\Xi(f)(s) \; := \; -\lim_{r \to 0} \frac{1}{\ln r} f \restriction_{\Gamma_r}(s)\,,
$$

$$
\Omega(f)(s) \; := \; \lim_{r \to 0} \left[f \restriction_{\Gamma_r}(s) + \Xi(f)(s)\ln r \right]\,,
$$

exist a.e. in $\mathbb{R}$, are independent of the direction $\frac{1}{r}(\xi,\eta)$, and define functions from $L^2(\mathbb{R})$

The case $\operatorname{codim}\Gamma = 2$

The restriction of $f \in W^{2,2}_{\text{loc}}(\mathbb{R}^3 \setminus \Gamma)$ to Γ_r is well defined for small r; we say that $f \in W^{2,2}_{\text{loc}}(\mathbb{R}^3 \setminus \Gamma) \cap L^2(\mathbb{R}^3)$ belongs to Υ if

$$\Xi(f)(s) := -\lim_{r \to 0} \frac{1}{\ln r} f \restriction_{\Gamma_r}(s),$$

$$\Omega(f)(s) := \lim_{r \to 0} \left[f \restriction_{\Gamma_r}(s) + \Xi(f)(s) \ln r \right],$$

exist a.e. in $\mathbb{R}$, are independent of the direction $\frac{1}{r}(\xi, \eta)$, and define functions from $L^2(\mathbb{R})$

Then the operator $H_{\alpha,\Gamma}$ has the domain

$$\{ g \in \Upsilon : 2\pi\alpha\Xi(g)(s) = \Omega(g)(s) \}$$

and acts as

$$-H_{\alpha,\Gamma} f = -\Delta f \quad \text{for} \quad x \in \mathbb{R}^3 \setminus \Gamma$$

Geometrically induced spectrum

Bending means *binding*, that is, it may create isolated eigenvalues of $H_{\alpha,\Gamma}$. Consider a *piecewise C^1-smooth* $\Gamma : \mathbb{R} \to \mathbb{R}^2$ parameterized by its arc length, and assume:

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- $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$ holds for some $c \in (0, 1)$

- Γ is *asymptotically straight*: there are $d > 0$, $\mu > \frac{1}{2}$ and $\omega \in (0, 1)$ such that

$$1 - \frac{|\Gamma(s) - \Gamma(s')|}{|s - s'|} \leq d \left[1 + |s + s'|^{2\mu}\right]^{-1/2}$$

in the sector $S_\omega := \left\{ (s, s') : \omega < \frac{s}{s'} < \omega^{-1} \right\}$

- *straight line is excluded*, i.e. $|\Gamma(s) - \Gamma(s')| < |s - s'|$ holds for some $s, s' \in \mathbb{R}$

Bending means binding

Theorem [E.-Ichinose'01]: Under these assumptions, $\sigma_{\text{ess}}(H_{\alpha,\Gamma}) = [-\frac{1}{4}\alpha^2, \infty)$ and $H_{\alpha,\Gamma}$ has *at least one eigenvalue* below the threshold $-\frac{1}{4}\alpha^2$

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- The same for *curves in* $\mathbb{R}^3$, under stronger regularity, with $-\frac{1}{4}\alpha^2$ is replaced by the corresponding 2D p.i. ev

- For *curved surfaces* $\Gamma \subset \mathbb{R}^3$ such a result is proved in the strong coupling asymptotic regime only

- *Implications for graphs:* let $\tilde{\Gamma} \supset \Gamma$ in the set sense, then $H_{\alpha,\tilde{\Gamma}} \leq H_{\alpha,\Gamma}$. If the essential spectrum threshold is the same for both graphs and Γ fits the above assumptions, we have $\sigma_{\text{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$ by minimax principle

Proof: generalized BS principle

Classical Birman-Schwinger principle based on the identity

$$(H_0 - V - z)^{-1} = (H_0 - z)^{-1} + (H_0 - z)^{-1} V^{1/2}$$

$$\times \left\{ I - |V|^{1/2}(H_0 - z)^{-1} V^{1/2} \right\}^{-1} |V|^{1/2}(H_0 - z)^{-1}$$

can be extended to generalized Schrödinger operators $H_{\alpha,\Gamma}$ [BEKŠ'94]: the multiplication by $(H_0 - z)^{-1} V^{1/2}$ etc. is replaced by suitable trace maps. In this way we find that $-\kappa^2$ is an eigenvalue of $H_{\alpha,\Gamma}$ *iff* the integral operator $\mathcal{R}_{\alpha,\Gamma}^{\kappa}$ on $L^2(\mathbb{R})$ with the kernel

$$(s, s') \mapsto \frac{\alpha}{2\pi} K_0 \left(\kappa |\Gamma(s) - \Gamma(s')| \right)$$

has an eigenvalue equal to one

Sketch of the proof

We treat $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ as a *perturbation* of the operator $\mathcal{R}^{\kappa}_{\alpha,\Gamma_0}$ referring to a *straight line*. The spectrum of the latter is found easily: it is *purely ac* and equal to $[0, \alpha/2\kappa)$

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The curvature-induced perturbation is *sign-definite*: we have $\left(\mathcal{R}^\kappa_{\alpha,\Gamma} - \mathcal{R}^\kappa_{\alpha,\Gamma_0} \right)(s, s') \geq 0$, and the inequality is sharp somewhere unless Γ is a straight line. Using a *variational argument* with a suitable trial function we can check the inequality $\sup \sigma(\mathcal{R}^\kappa_{\alpha,\Gamma}) > \frac{\alpha}{2\kappa}$

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Due to the assumed asymptotic straightness of Γ the perturbation $\mathcal{R}_{\alpha,\Gamma}^{\kappa} - \mathcal{R}_{\alpha,\Gamma_0}^{\kappa}$ is *Hilbert-Schmidt*, hence the spectrum of $\mathcal{R}_{\alpha,\Gamma}^{\kappa}$ in the interval $(\alpha/2\kappa, \infty)$ is discrete

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To conclude we employ continuity and $\lim_{\kappa \to \infty} \|\mathcal{R}^\kappa_{\alpha,\Gamma}\| = 0$. The argument can be pictorially expressed as follows:

# Pictorial sketch of the proof
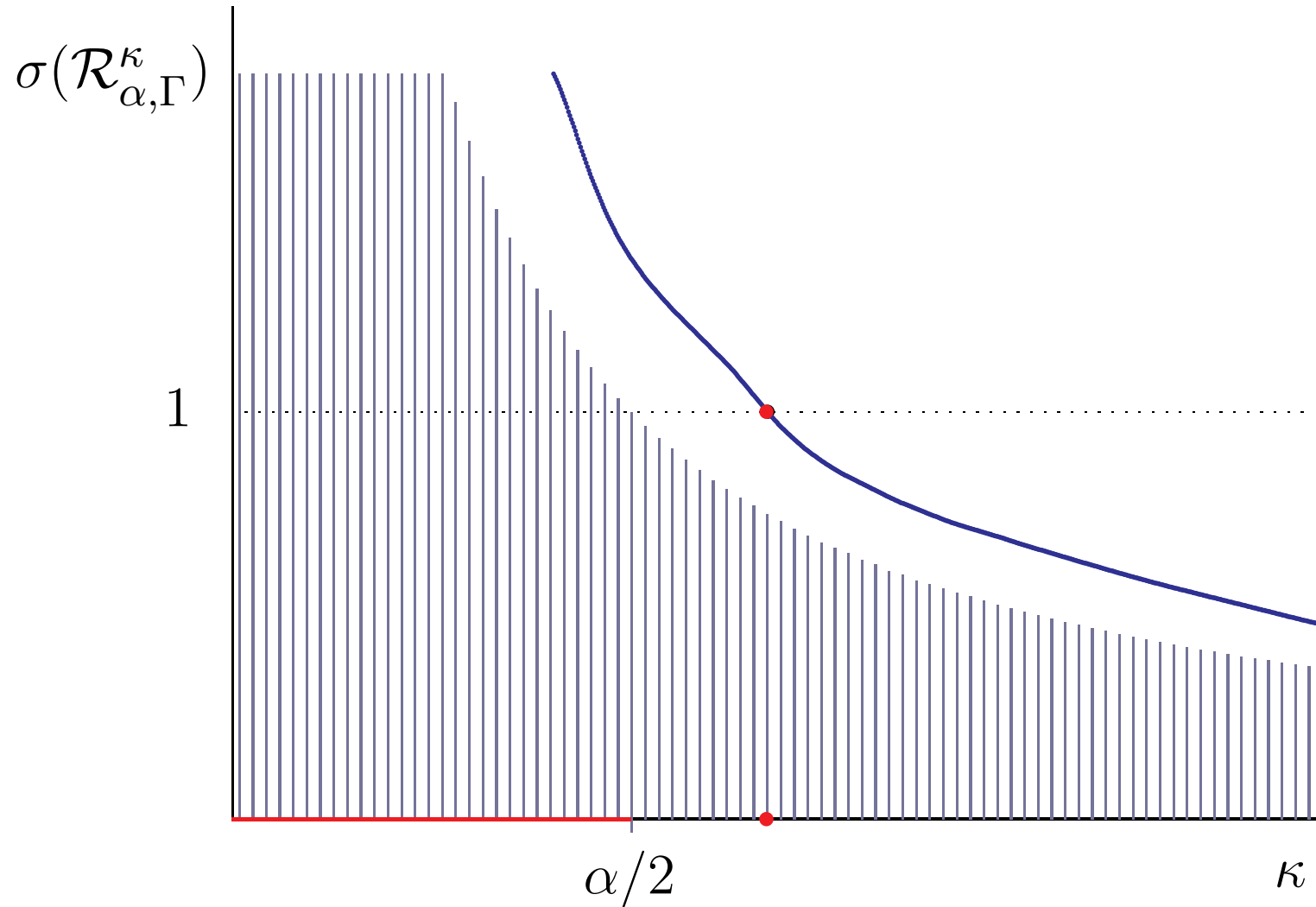
Other geometric perturbations

Consider now *perturbation theory for punctured manifolds:* a natural question is what happens with $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma})$ if Γ has a small *"hole"*. We will give the answer for a compact, $(n-1)$-dimensional, $C^{1+[n/2]}$-smooth manifold in $\mathbb{R}^n$

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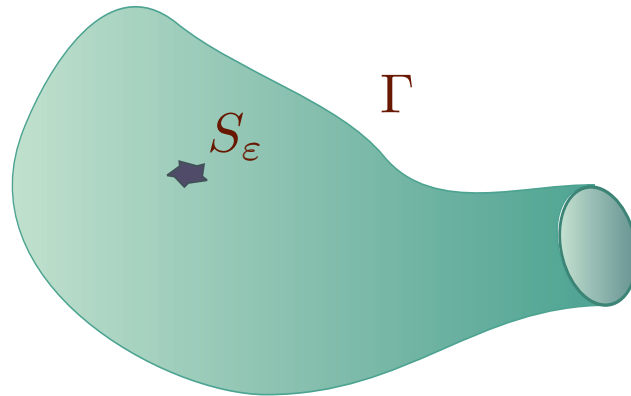
Consider a family $\{S_\varepsilon\}_{0\le\varepsilon<\eta}$ of subsets of Γ such that

- each S_ε is *Lebesgue measurable* on Γ

- they shrink to origin, $\sup_{x\in S_\varepsilon}|x| = \mathcal{O}(\varepsilon)$ as $\varepsilon\to 0$

- $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \ne \emptyset$, nontrivial for $n\ge 3$

Punctured manifolds: ev asymptotics

Call $H_\varepsilon := H_{\alpha, \Gamma \backslash S_\varepsilon}$. For small enough ε these operators have the same finite number of eigenvalues, naturally ordered, which satisfy $\lambda_j(\varepsilon) \to \lambda_j(0)$ as $\varepsilon \to 0$

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Let φ_j be the eigenfunctions of H_0. By Sobolev trace thm $\varphi_j(0)$ makes sense. Put $s_j := |\varphi_j(0)|^2$ if $\lambda_j(0)$ is simple, otherwise they are ev's of $C := \left(\overline{\varphi_i(0)} \varphi_j(0) \right)$ corresponding to a degenerate eigenvalue

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Theorem [E-Yoshitomi'03]: Under the assumptions made about the family $\{S_\varepsilon\}$, we have

$$\lambda_j(\varepsilon) = \lambda_j(0) + \alpha s_j m_\Gamma(S_\varepsilon) + o(\varepsilon^{n-1}) \quad \text{as} \quad \varepsilon \to 0$$

Remarks

- Formally a small-hole perturbation acts as a *repulsive δ interaction* with the coupling $\alpha m_\Gamma(S_\varepsilon)$

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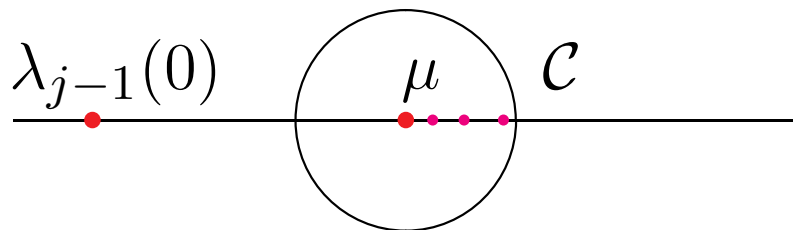
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- For *a curve in $\mathbb{R}^3$* we have a similar result, but the asymptotics is different [E.-Kondej'08]

$$\lambda_j(\varepsilon) = \lambda_j(0) + \omega(\lambda_j) s_j \varepsilon \ln \varepsilon + o(\varepsilon \ln \varepsilon) \quad \text{as} \quad \varepsilon \to 0$$
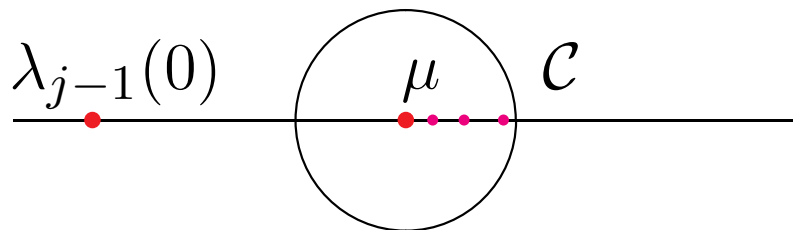
Proof sketch for $\operatorname{codim}\Gamma = 1$

Take an eigenvalue $\mu \equiv \lambda_j(0)$ of multiplicity m. It splits in general, for small enough ε one has m eigenvalues inside $\mathcal{C} := \{z : |z - \mu| < \frac{3}{4}\kappa\}$, where $\kappa := \frac{1}{2}\operatorname{dist}(\{\mu\}, \sigma(H_0) \setminus \{\mu\})$

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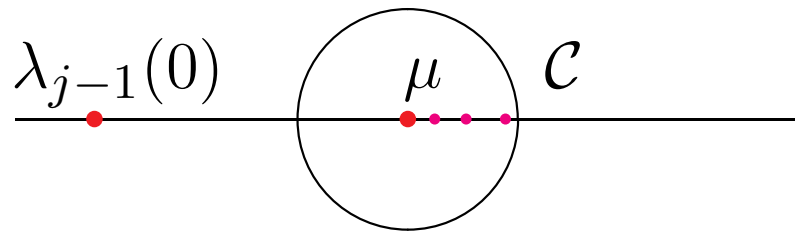$$\lambda_{j-1}(0) \qquad \mu \quad \mathcal{C}$$

Set $w_k(\zeta, \varepsilon) := (H_\varepsilon - \zeta)^{-1}\varphi_k - (H_0 - \zeta)^{-1}\varphi_k$ for $\zeta \in \mathcal{C}$ and $k = j, j+1, \ldots, j+m-1$. Using the choice of $\mathcal{C}$ and Sobolev imbedding thm, one proves

$$\|w_k(\zeta, \varepsilon)\|_{W^{1,2}(\mathbb{R}^n)} = \mathcal{O}(\varepsilon^{(n-1)/2}) \qquad \mathrm{as} \quad \varepsilon \to 0$$

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Next, $W^{1,2}(\mathbb{R}^n) \ni f \mapsto f|_\Gamma \in L^2(\Gamma)$ is compact; it implies

$$\sup_{\zeta \in \mathcal{C}} \|w_k(\zeta, \varepsilon)\|_{W^{1,2}(\mathbb{R}^n)} = o(\varepsilon^{(n-1)/2}) \quad \text{as} \quad \varepsilon \to 0$$

Proof sketch, continued

Let P_ε be spectral projection to these eigenvalues,

$$P_\varepsilon \varphi_k - \varphi_k = \frac{1}{2\pi i} \oint_{\mathcal{C}} w_k(\zeta, \varepsilon) \, d\zeta = o(\varepsilon^{(n-1)/2})$$

in $W^{1,2}(\mathbb{R}^n)$ as $\varepsilon \to 0$

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Take $m \times m$ matrices $L(\varepsilon) := ((H_\varepsilon P_\varepsilon \varphi_i, P_\varepsilon \varphi_k))$ and $M(\varepsilon) := ((P_\varepsilon \varphi_i, P_\varepsilon \varphi_k))$. We find that

$$((H_\varepsilon P_\varepsilon \varphi_i, P_\varepsilon \varphi_k)) - \mu \delta_{ik} - \alpha \overline{\varphi_i(0)} \varphi_k(0) m_\Gamma(S_\varepsilon)$$

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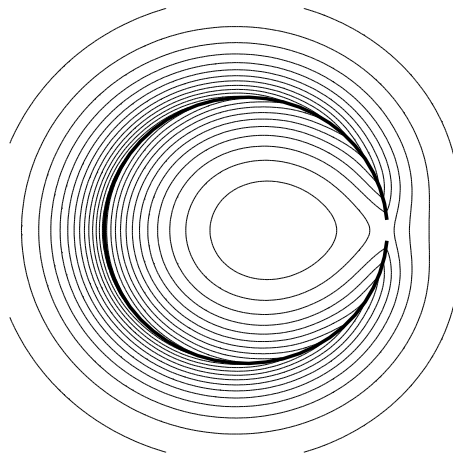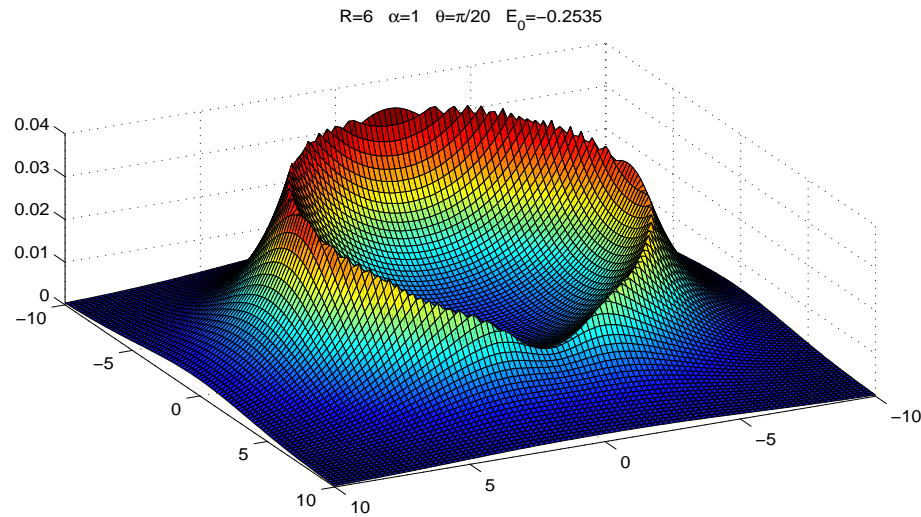
is $o(\varepsilon^{n-1})$ and $(P_\varepsilon \varphi_i, P_\varepsilon \varphi_k) = \delta_{ik} + o(\varepsilon^{n-1})$. Then

$$L(\varepsilon) M(\varepsilon)^{-1} = \mu I + \alpha C m_\Gamma(S_\varepsilon) + o(\varepsilon^{n-1})$$

and the claim of the theorem follows $\quad\square$

Illustration: a ring with $\frac{\pi}{20}$ cut

R=6 α=1 θ=π/20 E_0=−0.2535

Summarizing Lecture IV

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- *Bent edges* exhibit effective attractive interaction, *hiatus-type* perturbation give rise to a local repulsion

Some literature to Lecture IV

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- [E08] P.E.: Leaky quantum graphs: a review, AMS "Proceedings of Symposia in Pure Mathematics" Series, vol. 77, Providence, R.I., 2008; pp. 523-564.