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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- We will also look into the *high-energy behaviour* and show that there are situations when the asymptotics does not follow the Weyl law.
- 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 $\Gamma$ and spectral properties of a Schrödinger operator supported by $\Gamma$. An interpretation needed: think of $\Gamma$ 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 $\delta$-coupling of a strength $\alpha \neq 0$. 

![Diagram](image.png)
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 $\Gamma$ 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 $\Gamma_0$ can be treated as a periodic system analyzing the spectrum of the elementary cell with Floquet-Bloch boundary conditions with the phase $e^{2\beta \theta}$
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This yields the condition

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

$$\left| \cosh \kappa \pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa \pi}{\kappa} \right| = 1$$
Proposition, cont’d: The upper edge of this band depends on $\alpha$. 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 $\kappa$ 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 $\alpha$, in addition one has here the *infinitely degenerate point spectrum*.
- It is also an example of *gaps coming from decoration*. 
Now we pass to the bent chain denoted as $\Gamma_{\vartheta}$:
The bent chain spectrum

Now we pass to the bent chain denoted as $\Gamma_\vartheta$:

Since $\Gamma_\vartheta$ has mirror symmetry, the operator $H_\vartheta$ can be reduced by parity subspaces into a direct sum of an even part, $H^+$, and odd one, $H^-$; we drop mostly the subscript $\vartheta$.

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 linear combinations of $e^{\pm \beta k x}$,

$$
\psi_j(x) = C_j^+ e^{\beta k x} + C_j^- e^{-\beta k x}, \quad x \in [0, \pi],
\varphi_j(x) = D_j^+ e^{\beta k x} + D_j^- e^{-\beta k x}, \quad x \in [0, \pi]
$$

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

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\psi_0(x) = C_0^+ e^{\beta k x} + C_0^- e^{-\beta k x}, \quad x \in \left[\frac{\pi - \vartheta}{2}, \pi\right],
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$$

There are $\delta$-couplings in the points of contact, i.e.

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

$$
\psi_j(0) = \psi_{j-1}(\pi); \quad \psi_j'(0) + \varphi_j'(0) - \psi_{j-1}'(\pi) - \varphi_{j-1}'(\pi) = \alpha \cdot \psi_j(0)
$$
Using the above relations we get for all \( j \geq 2 \)

\[
\begin{pmatrix}
C^+_j \\
C^-_j
\end{pmatrix}
= \begin{pmatrix}
(1 + \frac{\alpha}{4\beta k}) e^{\beta k \pi} & \frac{\alpha}{4\beta k} e^{-\beta k \pi} \\
-\frac{\alpha}{4\beta k} e^{\beta k \pi} & (1 - \frac{\alpha}{4\beta k}) e^{-\beta k \pi}
\end{pmatrix}
\cdot
\begin{pmatrix}
C^+_{j-1} \\
C^-_{j-1}
\end{pmatrix},
\]
Transfer matrix

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\end{pmatrix}
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\end{pmatrix}

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;
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recall that reversed inequality characterizes spectral bands
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Remark: By general arguments, $\sigma_{\text{ess}}$ 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,

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

and an analogous expression for negative energies
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and an analogous expression for negative energies.

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 $\kappa_0$ 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,

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

and a similar one, with $\sin$ and $\cos$ replaced by $\sinh$ and $\cosh$ for negative energies.
Spectrum of $H^-$

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

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and a similar one, with $\sin$ and $\cos$ replaced by $\sinh$ and $\cosh$ for negative energies.

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, \( \alpha = -3 \)
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. In the above pictures their real parts are drawn as functions of \( \vartheta \) by dashed lines.
Resonances, analyticity

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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 $(\vartheta, k) = \left(\frac{n+1-2\ell}{n}\pi, n\right)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}_0$, $\ell \leq \left\lfloor \frac{n+1}{2} \right\rfloor$. 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 where 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 its vicinity we have

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

so the 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

We note that resonances in the example came from perturbations of embedded eigenvalues. Let us look at this problem in more generality:

- 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
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- \textit{Different resonances definitions:} poles of continued resolvent, singularities of on-shell S matrix
- Graphs may exhibit embedded eigenvalues due to invalidity of uniform continuation
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- Most typical resonance situations arise for *finite graphs with semiinfinite leads*

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

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

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

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

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

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

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

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

The Hamiltonian acts as $-d^2/dx^2$ 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 a “flower-like” graph with one vertex by putting all the vertices to a single point,

\[
\begin{align*}
  l_3 & \quad l_2 \\
  l_4 \quad l_1 \\
  l_N
\end{align*}
\]

Its degree is \(2N + M\) where \(N := \text{card } \mathcal{L}\) and \(M := \text{card } \mathcal{L}_\infty\)
A universal setting for graphs with leads

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

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 $\Gamma$. 
Equivalence of resonance definitions

Resonances as poles of analytically continued resolvent, \((H - \lambda \text{id})^{-1}\). 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 \(g_{j\theta}(x) = e^{\theta/2} g_j(xe^{\theta})\) with an imaginary \(\theta\) rotating the essential spectrum into the lower complex half-plane so that the poles of the resolvent on the second sheet become “uncovered” for \(\theta\) large enough. The “exterior” boundary values are thus equal to

\[g_j(0) = e^{-\theta/2} g_{j\theta}, \quad g'_j(0) = i k e^{-\theta/2} g_{j\theta}\]
Resolvent resonances

Substituting into the boundary conditions we get

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

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

\[C_1^{(j)}(k) = \begin{pmatrix} 0 & 1 \\ \sin kl_j & \cos kl_j \end{pmatrix}, \quad C_2^{(j)}(k) = \begin{pmatrix} 1 & 0 \\ -\cos kl_j & \sin kl_j \end{pmatrix}\]
In this case we choose a combination of two planar waves, $g_j = c_j e^{-ikx} + d_j e^{ikx}$, 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 $d = Sc$. 
Scattering resonances

In this case we choose a combination of two planar waves, $g_j = c_j e^{-ikx} + d_j e^{ikx}$, 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 $d = Sc$. The b.c. give

$$(U - I)C_1(k) \begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ c_1 + d_1 \\ \vdots \\ c_M + d_M \end{pmatrix} + ik(U + I)C_2(k) \begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ d_1 - c_1 \\ \vdots \\ d_M - c_M \end{pmatrix} = 0$$
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 \textit{not} solvable, $\det S^{-1} = 0$, if

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

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

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 \textit{with compactly supported eigenfunctions}; they are embedded in the continuum corresponding to external semiinfinite edges.
Embedded eigenvalues

**Theorem [E-Lipovský’10]:** Let $\Gamma$ 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 $M_{\text{even}}$ 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 $M_{\text{even}}$. 

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

\[
\begin{align*}
    f_1(0) &= f_2(0), \\
    f_1(l_1) &= f_2(l_2), \\
    f_1(0) &= \alpha_1^{-1}(f'_1(0) + f'_2(0)) + \gamma_1 g'_1(0), \\
    f_1(l_1) &= -\alpha_2^{-1}(f'_1(l_1) + f'_2(l_2)) + \gamma_2 g'_2(0), \\
    g_1(0) &= \tilde{\gamma}_1(f'_1(0) + f'_2(0)) + \tilde{\alpha}_1^{-1} g'_1(0), \\
    g_2(0) &= -\tilde{\gamma}_2(f'_1(l_1) + f'_2(l_2)) + \tilde{\alpha}_2^{-1} g'_2(0)
\end{align*}
\]
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 $\lambda$ 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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where $\beta^{-1}_i(k) := \alpha_i^{-1} + \frac{ik|\gamma_i|^2}{1-ik\tilde{\alpha}_i^{-1}}$.

The condition can be solved numerically to find the resonance trajectories with respect to the variable $\lambda$. 

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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 $\lambda$ changing from red ($\lambda = 0$) to blue ($\lambda = 1$).
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.
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

\[ g_1(x) \quad f_1(x) \quad l_1 = l (1 - \lambda) \]

\[ g_2(x) \quad f_2(x) \quad l_2 = l (1 + \lambda) \]

\[ l_1 = l (1 - \lambda) \]

\[ l_2 = l (1 + \lambda) \]
Example: a cross-shaped graph

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

\[
\begin{align*}
  f_1(0) & = f_2(0) = g_1(0) = g_2(0), \\
  f_1(l_1) & = f_2(l_2) = 0, \\
  \alpha f_1(0) & = f'_1(0) + f'_2(0) + g'_1(0) + g'_2(0).
\end{align*}
\]

leading to the resonance condition

\[
2k \sin 2kl + (\alpha - 2ik)(\cos 2kl\lambda - \cos 2kl) = 0
\]
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.
The trajectory of the resonance pole for the coefficients values $\alpha = 1$, $n = 2$. The colour coding is the same as above.
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 $\Gamma$ 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 $\det[(1 - k_0)U_4 - (1 + k_0)I] \neq 0$ be a pole of the resolvent $(H - \lambda \text{id})^{-1}$ of a multiplicity $d$. Let $\Gamma_\varepsilon$ 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 $\varepsilon \in \mathcal{U}_{\varepsilon_0}(0)$ the sum of multiplicities of the resolvent poles in a sufficiently small neighbourhood of $k_0$ is $d$. 
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Let \( k_0 \) satisfying \( \det \left[ (1 - k_0)U_4 - (1 + k_0)I \right] \neq 0 \) be a pole of the resolvent \( (H - \lambda I)^{-1} \) of a multiplicity \( d \). Let \( \Gamma_\varepsilon \) 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 \( \varepsilon \in \mathcal{U}_{\varepsilon_0}(0) \) 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 \( \varepsilon \) 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. If $F$ comes from resonance secular equation we count in this way number of resonances within the given circle
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If $F$ comes from resonance secular equation we count in this way *number of resonances* within the given circle.

They made an intriguing observation: if the coupling is *Kirchhoff* and some external vertices are *balanced*, i.e. connecting the same number of internal and external edges, then the leading term in the asymptotics may be *less than Weyl formula prediction*.
And another resonance problem

The paper [DET’08] also inspired [Davies-Pushnitski’10] who looked into \textit{high-energy asymptotics} of graph resonances. As usual \textit{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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They made an intriguing observation: if the coupling is \textit{Kirchhoff} and some external vertices are \textit{balanced}, i.e. connecting the same number of internal and external edges, then the leading term in the asymptotics may be \textit{less than Weyl formula prediction}.

Let us look how the situation looks like for graphs with \textit{more general vertex couplings}.
Recall the resonance condition

Denote \( e_j^\pm := e^{\pm ikl_j} \) and \( e^\pm := \prod_{j=1}^{N} e_j^\pm \), then secular eq-n is

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

where \( E_i(k) = \text{ diag } \left( E_i^{(1)}, E_i^{(2)}, \ldots, E_i^{(N)}, 0, \ldots, 0 \right) \), \( i = 1, 2, 3, 4 \), consists of \( N \) nontrivial \( 2 \times 2 \) 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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+ (U-I) E_4 + [(U-I) - k(U+I)] \text{diag} (0, \ldots, 0, I_{M \times M}) \right\},$$

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

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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 \( F(k) = \sum_{r=0}^{n} a_r(k) e^{ik\sigma_r} \), 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 \( \Omega \) lie in the logarithmic strips bounded by the curves \( -\text{Im } k + m_r \log |k| = \pm K_r \) 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,

\[
0 = \det \left\{ \frac{1}{2} [(\tilde{U}(k) - I) + k(\tilde{U}(k) + I)]\tilde{E}_1(k) \right.
\]

\[
+ \frac{1}{2} [(\tilde{U}(k) - I) - k(\tilde{U}(k) + I)]\tilde{E}_2(k) + k(\tilde{U}(k) + I)\tilde{E}_3 + (\tilde{U}(k) - I)\tilde{E}_4 \right\},
\]

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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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

$$\left( \frac{i}{2} \right)^N \det [(\tilde{U}(k) - I) \pm k(\tilde{U}(k) + I)]$$
The resonance asymptotics

**Theorem** [Davies-E-Lipovský’10]: Consider a quantum graph \((\Gamma, H_U)\) corresponding to \(\Gamma\) with finitely many edges and the coupling at vertices \(x_j\) given by unitary matrices \(U_j\). The asymptotics of the resonance counting function as \(R \to \infty\) is of the form

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

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 $|b_j + a_j \deg X_j| = 1$; matrix $J$ has all entries equal to one.

Note that $\delta$ and $\delta'_s$ are particular cases of such a coupling.
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We need two simple auxiliary statements:

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

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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.
Asymptotics in the symmetric case

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**Theorem** [Davies-E-Lipovský’10]: Let \((\Gamma, H_U)\) 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 $W_4$,

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

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 $W^{-1}UW$. 

Unbalanced non-Weyl graphs
Example: line with a stub

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

$$0 = (U - I) (u(0), f_1(0), f_2(0))^T + i(U + I) (u'(0), f_1'(0), f_2'(0))^T,$$

$$0 = u(l) + cu'(l),$$

$f_i(x)$ 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).
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)

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

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

\[
U = \begin{pmatrix} 0 & \text{re}^{i\varphi_1} & \sqrt{1-r^2}\text{e}^{i\varphi_2} \\ \text{re}^{-i\varphi_1} & (1-r^2)\text{e}^{i\psi} & -r\sqrt{1-r^2}\text{e}^{-i(-\psi+\varphi_1-\varphi_2)} \\ \sqrt{1-r^2}\text{e}^{-i\varphi_2} & -r\sqrt{1-r^2}\text{e}^{i(\psi+\varphi_1-\varphi_2)} & r^2\text{e}^{i\psi} \end{pmatrix}
\]
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 $x_1$ 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 $\Gamma_0$, 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.
**Proposition:** Consider $\Gamma$ be the the coupling given by arbitrary $U^{(1)}$ and $U^{(2)}$. Let $V$ be an arbitrary unitary $p \times p$ matrix, $V^{(1)} := \text{diag} (V, V)$ and $V^{(2)} := \text{diag} (I_{(q-p) \times (q-p)}, V)$ be $2p \times 2p$ and $q \times q$ block diagonal matrices, respectively. Then $H$ on $\Gamma$ 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 $[V^{(2)}]^{-1}U^{(2)}V^{(2)}$. 
Unitary equivalence again

**Proposition:** Consider $\Gamma$ be the coupling given by arbitrary $U^{(1)}$ and $U^{(2)}$. Let $V$ be an arbitrary unitary $p \times p$ matrix, $V^{(1)} := \text{diag}(V, V)$ and $V^{(2)} := \text{diag}(I_{(q-p)\times(q-p)}, V)$ be $2p \times 2p$ and $q \times q$ block diagonal matrices, respectively. Then $H$ on $\Gamma$ 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 $[V^{(2)}]^{-1}U^{(2)}V^{(2)}$.

**Remark:** The assumption that the same edge length is made for convenience only; we can always get it fulfilled by adding Kirchhoff vertices.
Application to symmetric coupling

Let now $U^{(1)} = aJ_{2p \times 2p} + bI_{2p \times 2p}$ at $x_1$. 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 $\frac{1}{\sqrt{p}} (1, 1, \ldots, 1)^T$. The transformed matrix $[V^{(1)}]^{-1} U^{(1)} V^{(1)}$ decouples into blocks connecting only pairs $(v_j, g_j)$. 
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 $\frac{1}{\sqrt{p}} (1, 1, \ldots, 1)^T$. The transformed matrix $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ decouples into blocks connecting only pairs $(v_j, g_j)$.

The first one corresponding to a symmetrization of all the $u_j$'s and $f_j$'s, leads to the $2 \times 2$ 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 $j = 2, \ldots, p$. 
Application to symmetric coupling

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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

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:

For a fixed integer \( n \geq 3 \) we start with a regular \( n \)-gon, each edge having length \( \ell \), 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 $\Gamma_n$ is given by

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

Proposition: The effective size of the graph $\Gamma_n$ is given by

$$W_n = \begin{cases} 
  n\ell/2 & \text{if } n \not\equiv 0 \pmod{4}, \\
  (n - 2)\ell/2 & \text{if } n \equiv 0 \pmod{4}.
\end{cases}$$

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” $\omega$ satisfying $\omega^n = 1$; after a short computation we find that $H\omega$ has a resonance iff

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

Hence the effective size $W_\omega$ of the system of resonances of $H_\omega$ 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 $n \not\equiv 0 \pmod{4}$, but it has two solutions if $n = 0 \pmod{4}$. □
Adding a magnetic field

Now the Hamiltonian acts as $-\frac{d^2}{dx^2}$ at the infinite leads and as $-(d/dx + iA_j(x))^2$ 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

$$(U_j - I)\Psi_j + i(U_j + I)(\Psi'_j + iA_j\Psi_j) = 0$$
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Using local gauge transformation \(\psi_j(x) \mapsto \psi_j(x)e^{-i\chi_j(x)}\) with \(\chi_j(x)' = A_j(x)\) one gets unitary equivalence to \textit{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 \(\mathcal{F} = \text{diag} \ (1, \exp (i\Phi_1), \ldots, 1, \exp (i\Phi_N), 1, \ldots, 1)\) containing magnetic fluxes \(\Phi_j = \int_0^{l_j} A_j(x) \, dx\)
Magnetic graph asymptotics

**Theorem [E-Lipovský’11]:** Let $\Gamma$ 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 $\Gamma_V$ be obtained from $\Gamma$ 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 $\Gamma_V$ has a non-Weyl resonance asymptotics iff $\Gamma$ does.

**Proof:** Using the effective coupling matrix $\tilde{U}(k)$ as in the non-magnetic case □
Theorem [E-Lipovský’11]: Let $\Gamma$ 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 $\Gamma_V$ be obtained from $\Gamma$ 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 $\Gamma_V$ has a non-Weyl resonance asymptotics iff $\Gamma$ does.

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

Corollary: Let $\Gamma$ be a quantum graph with Weyl resonance asymptotics. Then $\Gamma_A$ has also the Weyl asymptotics for any profile of the magnetic field.
The magnetic field can change, though, the effective size
Example

The magnetic field can change, though, the effective size

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

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

where $\Phi = Al$ is the loop flux. For $\Phi = \pm \pi/2 \ (\text{mod} \ \pi)$, odd multiples of a quarter of the flux quantum $2\pi$, 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.
Local geometric perturbations of quantum graphs can produce eigenvalues in gaps as well as resonances.
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Embedded eigenvalues of quantum graphs are generically unstable and can turn into resonances when the size ratios change.
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.
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


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.
Lecture overview

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

A model of "leaky" quantum wires and graphs, with Hamiltonians of the type $H_{\alpha,\Gamma} = -\Delta - \alpha \delta(x - \Gamma)$
Lecture overview

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

- A model of "leaky" quantum wires and graphs, with Hamiltonians of the type \( H_{\alpha, \Gamma} = -\Delta - \alpha \delta(x - \Gamma) \)

- Geometrically induced spectral bound states of leaky wires and graphs: bent edges
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- Why we might want *something better* than the ideal graph model of the previous lectures

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- *Geometrically induced spectral bound states* of leaky wires and graphs: bent edges

- 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.

As we have seen in *Lectures I, II* it is possible but not exactly easy, and some work remains to be done.
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.

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

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

in \( L^2(\mathbb{R}^2) \), where \( \Gamma \) is the graph in question.
Leaky quantum graphs

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

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in \( L^2(\mathbb{R}^2) \), where \( \Gamma \) is the graph in question.

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

\[ \psi \mapsto \||\nabla \psi\||^2_{L^2(\mathbb{R}^n)} - \alpha \int_{\Gamma} |\psi(x)|^2 \, dx, \]

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 \( \Gamma \).
Leaky graph Hamiltonians

For $\Gamma$ 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 $W^{2,1}_{\text{loc}}(\mathbb{R}^2 \setminus \Gamma)$, which are continuous and exhibit a normal-derivative jump,

$$\frac{\partial \psi}{\partial n}(x) \bigg|_+ - \frac{\partial \psi}{\partial n}(x) \bigg|_- = -\alpha \psi(x)$$
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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 $\text{codim} \Gamma$ does not exceed three
The case $\text{codim } \Gamma = 2$

Boundary conditions can be used but they are more complicated. Moreover, for an infinite $\Gamma$ corresponding to $\gamma : \mathbb{R} \to \mathbb{R}^3$ we have to assume in addition that there is a tubular neighbourhood of $\Gamma$ which does not intersect itself.
The case $\text{codim } \Gamma = 2$

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

Employ Frenet’s frame $(t(s), b(s), n(s))$ for $\Gamma$. 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 $\text{codim} \, \Gamma = 2$

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

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

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

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

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:
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:

- $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$ holds for some $c \in (0, 1)$
- $\Gamma$ 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 $S_\omega := \{(s, s') : \omega < \frac{s}{s'} < \omega^{-1}\}$
- 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, 
\[ \sigma_{\text{ess}}(H_{\alpha,\Gamma}) = \left[ -\frac{1}{4}\alpha^2, \infty \right) \] and \( H_{\alpha,\Gamma} \) has *at least one* eigenvalue below the threshold \( -\frac{1}{4}\alpha^2 \)
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and \( H_{\alpha,\Gamma} \) has **at least one** eigenvalue below the threshold \(-\frac{1}{4}\alpha^2\)

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

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

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

\[ \sigma(\mathcal{R}_{\alpha, \Gamma}^\kappa) \]

\[ 1 \]

\[ \frac{\alpha}{2} \]

\[ \kappa \]
Other geometric perturbations

Consider now *perturbation theory for punctured manifolds*: a natural question is what happens with \( \sigma_{\text{disc}}(H_\alpha, \Gamma) \) if \( \Gamma \) 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 $\{S_\varepsilon\}_{0 \leq \varepsilon < \eta}$ of subsets of $\Gamma$ such that

- each $S_\varepsilon$ is Lebesgue measurable on $\Gamma$,
- they shrink to origin, $\sup_{x \in S_\varepsilon} |x| = \mathcal{O}(\varepsilon)$ as $\varepsilon \to 0$,
- $\sigma_{\text{disc}}(H_\alpha, \Gamma) \neq \emptyset$, nontrivial for $n \geq 3$.
Punctured manifolds: ev asymptotics

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

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

Let \( \varphi_j \) 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 \( C := (\overline{\varphi_i(0)} \varphi_j(0)) \) corresponding to a degenerate eigenvalue
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Let $\varphi_j$ 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.

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

$$\lambda_j(\varepsilon) = \lambda_j(0) + \alpha s_j m_\Gamma(S_\varepsilon) + o(\varepsilon^{n-1}) \quad \text{as} \quad \varepsilon \to 0$$
Formally a small-hole perturbation acts as a \textit{repulsive} $\delta$ \textit{interaction} with the coupling $\alpha m \Gamma(S_\varepsilon)$.
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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 \textbf{codim} \( \Gamma = 1 \)

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

\[ \lambda_{j-1}(0) \quad \mu \quad \mathcal{C} \]
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![Diagram](image)

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

$$\|w_k(\zeta, \varepsilon)\|_{W^{1,2}(\mathbb{R}^n)} = \mathcal{O}(\varepsilon^{(n-1)/2}) \quad \text{as} \quad \varepsilon \to 0$$
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\[
\begin{array}{c}
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\end{array}
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\| w_k(\zeta, \varepsilon) \|_{W^{1,2}(\mathbb{R}^n)} = \mathcal{O}(\varepsilon^{(n-1)/2}) \quad \text{as} \quad \varepsilon \to 0
\]

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 $P_\varepsilon$ be spectral projection to these eigenvalues,

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

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

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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

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

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

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

and the claim of the theorem follows $\square$
Illustration: a ring with $\frac{\pi}{20}$ cut
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Summarizing Lecture IV

- **“Leaky” graphs** are a more realistic model of graph-like nanostructures because they take quantum tunneling into account.

- *Geometry plays essential role* in determining spectral and scattering properties of such systems.

- **Bent edges** exhibit effective attractive interaction, *hiatus-type* perturbation give rise to a local repulsion.
Some literature to Lecture IV


