# Introduction to quantum graphs and their resonance properties

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## 1 Introduction

Quantum graphs are quite a simple model which studies behaviour of a quantum particle on a network. First attempts to place a quantum particle to a graph date back to 1930's (Pauling [Pau36] studied diamagnetic properties of aromatic molecules) and 1950's (work of Ruedenberg and Scherr [RS53] on $\pi$-electron behavior in aromatic molecules). The model has been developed mainly in the last thirty years.

From a mathematical point of view this model is quite simple – it is a set of ordinary differential equations. Hence it can be used as a toy model for various notions. For instance, it has been used for study of quantum chaos [KS97]. Spectral and resonance properties of quantum graphs can be directly measured; quantum graph is simulated by a microwave network, see e.g. [HBP+04].

## 2 Description of the model

First, we consider a metric graph $\Gamma$. It consists of the set of vertices $\mathcal{X}_j$, the set of $N$ internal edges $\mathcal{E}_{\mathrm{i}}$ of positive lengths $l_j$ and set of $M$ infinite edges $\mathcal{E}_{\mathrm{e}}$ – halflines which can be parametrized by $[0,\infty)$. The Hilbert space of our system consists of functions with components square integrable on each edge

$$\mathcal{H} = \bigoplus_{i=1}^{N} L^2((0,l_i)) \oplus \bigoplus_{i=1}^{M} L^2((0,\infty))\,.$$

The vector in this Hilbert space is

$$\psi = (\psi_1, \ldots, \psi_N, \psi_{N+1}, \ldots, \psi_{N+M})^{\mathrm{T}}\,.$$

The whole structure is equipped with a second order operator, the Hamiltonian which acts as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$ with a bounded potential $V(x)$. Potential is located only on the internal edges. This Hamiltonian corresponds to a simplified Hamiltonian of a quantum particle $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$; we have chosen the set of units in which $\hbar = 1$ and $m = 1/2$. The domain of our Hamiltonian consists of functions in Sobolev space on the graph $W^{2,2}(\Gamma)$ (which is an orthogonal sum of Sobolev spaces on the edges). The function belongs to Sobolev space $W^{k,p}(e)$ on the edge $e$ if its weak derivatives up to the order $k$ belong to $L^p(e)$. Moreover, functions from the domain of the Hamiltonian must satisfy the coupling conditions at the vertices

$$(U_j - I)\Psi_j + i(U_j + I)\Psi_j' = 0\,, \tag{1}$$

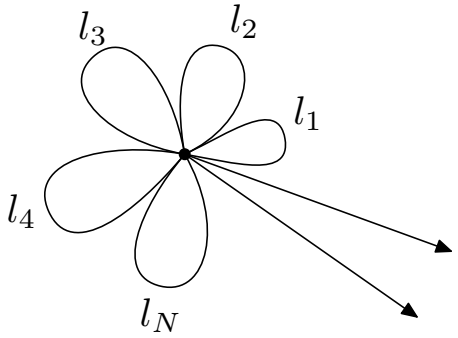


Figure 1: A flower-like graph

where $U_j$ is a $d_j \times d_j$ matrix, where $d_j$ is degree of $j$-th vertex, $I$ is $d_j \times d_j$ unit matrix, $\Psi_j$ is the vector of limits of functional values from various edges to the $j$-th vertex and, similarly, $\Psi'_j$ is the vector of outgoing derivatives.

The following construction can be used to describe easily the coupling on the whole graph. One joins all the vertices into one and obtains one-vertex "flower-like" graph (see figure 1). The coupling on the whole graph can be described by only one big unitary $(2N + M) \times (2N + M)$ matrix $U$ [Kuc08, EL10] with coupling condition

$$(U - I)\Psi + i(U + I)\Psi' = 0\,, \tag{2}$$

This matrix describes not only the coupling but also the topology of the graph. The flower-like model with eq. (2) will be equivalent to the multivertex graph with eq. (1) if we choose the matrix $U$ to be block-diagonal in the bases corresponding to the topology of the graph with blocks $U_j$.

# 3 Coupling condition and their derivation

In this section we prove that the equation (2) describes all possible selfadjoint Hamiltonians defined in the previous section.

**Definition 3.1.** *Let $L$ be an operator in the Hilbert space $\mathcal{H}$ with the scalar product $(\cdot, \cdot)$. By its adjoint we denote the operator $L^*$, which acts as $L^*y = y^*$, where $(y, Lx) = (y^*, x)$ for all $x \in D(L)$. The domain of $L^*$ consists of all $y$ for which the above relation holds. The operator is symmetric if $(y, Lx) = (Ly, x)$ and selfadjoint if $L = L^*$, i.e. the domains of $L$ and $L^*$ coincide. A selfadjoint operator $L_1$ is called selfadjoint extension if $D(L) \subset D(L_1)$ and $L = L_1$ on $D(L)$.*

There has been developed a theory how to construct selfadjoint extensions, but we will not reproduce it here. It can be found e.g. in the textbooks [BEH08, RS75]. We define a symmetric operator $H_0$ which acts as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_j(x)$ on the $j$-th edge of the flower-like graph, with domain consisting of functions in $W^{2,2}(\Gamma)$

for which both functional value and the derivative vanish at the central vertex. The domain of its adjoint is $W^{2,2}(\Gamma)$ without any coupling conditions at the central vertex.

We study the following skew-Hermitian form

$$\Omega(\phi,\psi) = -\overline{\Omega(\psi,\phi)} = (H_0^*\phi,\psi) - (\phi, H_0^*\psi)\,.$$

Using integration by parts one can find that

$$\begin{aligned}
\Omega(\phi,\psi) = \sum_{j=1}^{N+M} \int_{e_j} \Big[ &-\bar{\phi_j}''(x)\psi_j(x) + V_j(x)\bar{\phi_j}(x)\psi_j(x) - \\
&- \big(-\bar{\phi_j}(x)\psi_j''(x) + V_j(x)\bar{\phi_j}(x)\psi_j(x)\big)\Big]\,\mathrm{d}x = \\
&= \sum_{j=1}^{N+M} \int_{e_j} \Big(-\bar{\phi_j}''(x)\psi_j(x) + \bar{\phi_j}(x)\psi_j''(x)\Big) = \\
= \sum_{j=1}^{N+M} \Big(-\bar{\psi_j}'(0)\psi_j(0) + \bar{\phi_j}(0)\psi_j'(0)\Big) &+ \sum_{j=1}^{N} \Big(\bar{\phi_j}'(l_j)\psi_j(l_j) - \bar{\phi_j}(l_j)\psi_j'(l_j)\Big) - \\
&- \sum_{j=1}^{N+M} \int_{e_j} \Big(-\bar{\phi_j}'(x)\psi_j'(x) + \bar{\phi_j}'(x)\psi_j'(x)\Big)\,\mathrm{d}x = \\
&= \Phi^*\Psi' - \Phi'^*\Psi = \omega([\Phi],[\Psi]) = ([\Phi],\mathcal{J}[\Psi])_{\mathbb{C}^{4N+2M}}\,.
\end{aligned}$$

where $e_j$, $j = 1,\dots,N$ are internal edges and $j = N+1,\dots,N+M$ are external edges, $\mathcal{J} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ and vectors $[\Phi] = (\Phi,\Phi')^{\mathrm{T}}$, $[\Psi] = (\Psi,\Psi')^{\mathrm{T}}$ contain limits of functional values and derivatives in the central vertex. The star in the last line of the equation denotes transposition and complex conjugation.

**Definition 3.2.** *Let $W$ be a subspace of $\mathbb{C}^{4N+2M}$. We denote by $W^\perp = \{[\Psi] \in \mathbb{C}^{4N+2M} : \omega([\Psi],[\Phi]) = 0, \forall [\Phi] \in W\}$. We call the subspace $W$ maximal isotropic or a Lagrangian plane if $W^\perp = W$.*

Now we prove the theorem on the coupling conditions. It has been independently proven by Kostrykin and Schrader [KS99] and Harmer [Har00]. In the proof of the theorem we use the simple argument from [FT00] originally based on physical reasons.

**Theorem 3.3.** *All selfadjoint extensions of the operator $H_0$ can be uniquely parametrized by the set of unitary matrices $U$ of rank $(2N+M)\times(2N+M)$ by the equation (2).*

*Proof.* We will prove that the subspace is a Lagrangian plane if and only if it is parametrized by the equation (2). First, we prove that every Lagrangian plane is parametrized by equation (2). Necessary condition for $\omega([\Phi],[\Psi]) = 0$ for

all $[\Phi], [\Psi] \in W$ is $\omega([\Phi],[\Phi]) = 0$ for all $[\Phi] \in W$. Let us now compute the following expression

$$\begin{aligned}
&\|\Phi + i\Phi'\|^2_{\mathbb{C}^{2N+M}} - \|\Phi - i\Phi'\|^2_{\mathbb{C}^{2N+M}} = \\
&\qquad = (\Phi + i\Phi', \Phi + i\Phi')_{\mathbb{C}^{2N+M}} - (\Phi - i\Phi', \Phi - i\Phi')_{\mathbb{C}^{2N+M}} = \\
&\quad = \Phi^*\Phi - i\Phi'^*\Phi + i\Phi^*\Phi' + \Phi'^*\Phi' - \Phi^*\Phi - i\Phi'^*\Phi + i\Phi^*\Phi' - \Phi'^*\Phi' = \\
&\qquad\qquad = 2i[\Phi^*\Phi' - \Phi'^*\Phi] = 2i\omega([\Phi],[\Phi]) = 0\,.
\end{aligned}$$

Hence the norm of the vectors $\Phi + i\Phi'$ and $\Phi - i\Phi'$ must be the same and these vectors must be related by a unitary matrix $U$. From the equation $U(\Phi + i\Phi') = \Phi - i\Phi'$ follows the equation (2).

Now we prove that every subspace parametrized by (2) is a Lagrangian plane. We notice that the form $\omega$ can be rewritten as

$$\begin{aligned}
&\omega([\Phi],[\Psi]) = (\Phi^*, \Phi'^*) \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \Psi \\ \Psi' \end{pmatrix} = \\
&= (\Phi^*, \Phi'^*) \begin{pmatrix} V^{-1} & 0 \\ 0 & V^{-1} \end{pmatrix} \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} V^{-1} & 0 \\ 0 & V^{-1} \end{pmatrix} \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} \Psi \\ \Psi' \end{pmatrix} = \\
&\qquad = ((V\Phi)^*, (V\Phi')^*) \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} V\Psi \\ V\Psi' \end{pmatrix},
\end{aligned}$$

where $V$ is a $(2N + M) \times (2N + M)$ unitary matrix. Since we can rewrite the equation (2) as

$$V^{-1}(D - I)V\Psi + iV^{-1}(D + I)V\Psi' = 0\,,$$

where $D$ is a $(2N + M) \times (2N + M)$ diagonal unitary matrix, it suffices to prove it only for diagonal matrices. If $D$ does not have eigenvalues $-1$, we obtain from the previous equation $V\Psi' = i(D + I)^{-1}(D - I)V\Psi$, $(V\Phi')^* = (V\Phi)^*(-i)(D^* - I)(D^* + I)^{-1}$ and consequently

$$\omega([\Phi],[\Psi]) = ((V\Phi)^*, (V\Phi)^*) \begin{pmatrix} 0 & i(D + I)^{-1}(D - I) \\ i(D^* - I)(D^* + I)^{-1} & 0 \end{pmatrix} \begin{pmatrix} V\Psi \\ V\Psi \end{pmatrix}.$$

From the unitary properties of $D$ we have

$$(D+I)(D^*-I)+(D-I)(D^*+I) = DD^*-D+D^*-I+DD^*-D^*+D-I = 0$$

and hence for no eigenvalue -1

$$(D^* - I)(D^* + I)^{-1} + (D + I)^{-1}(D - I) = 0\,.$$

Therefore, the form $\omega$ vanishes

$$\omega([\Phi],[\Psi]) = iV\Phi^*[(D^* - I)(D^* + I)^{-1} + (D + I)^{-1}(D - I)]V\Psi = 0$$

for every $[\Phi]$, $[\Psi]$ satisfying (2). If $D$ has eigenvalues $-1$, from the coupling condition follows that entries of $V\Psi$ and $V\Phi$ corresponding to these eigenvalues vanish. In the subspace corresponding to other eigenvalues, previous argument can be used. □

**Remark 3.4.** *Condition* $\omega([\Phi],[\Phi]) = \Phi^*\Phi' - \Phi'^*\Phi = 0$ *has a simple physical interpretation. It means that the probability current* $j = \frac{\hbar}{2mi}(\bar{\phi}\phi' - \bar{\phi}'\phi)$ *through the central vertex is conserved. We could have used in the difference* $\|\Phi + il\Phi'\|^2 - \|\Phi - il\Phi'\|^2$ *with* $l \in \mathbb{R}$ *in the proof and obtain the coupling condition* $(U-I)\Psi + il(U+I)\Psi' = 0$*, but this equation can be related to an equivalent form* $(U_1 - I)\Psi + i(U_1 + I)\Psi' = 0$ *and hence does not add any degree of freedom. The choice of* $l$ *just fixes the length scale.*

**Remark 3.5.** *If we start from the flower-like graph and obtain coupling condition (2), we have for the corresponding multivertex graph a coupling conditions which allow for "hopping" particle between vertices. If we want to get rid of it, we need to choose the coupling matrix* $U$ *to be block diagonal with respect to the topology of the graph.*

Now we describe the most common coupling conditions.

- **permutation symmetric coupling conditions**
  This type of the condition is symmetric to the change of any two leads emanating from the vertex. The unitary matrix is $U = aJ + bI$, where $J$ has all entries equal to one and $a$ and $b$ are complex constants. Using $J^2 = nJ$ ($n$ is a degree of a vertex) and $JI = IJ = J$ and unitarity of the coupling matrix we have

  $$|a|^2 nJ + b\bar{a}J + a\bar{b}J + |b|^2 I = I\,. \tag{3}$$

  From this we can obtain that $|b| = 1$ and $|an + b| = 1$. The first relation obviously follows from the previous equation, the proof of the second one is following

  $$|an+b|^2 = |a|^2 n^2 + \bar{a}bn + a\bar{b}n + |b|^2 = n(|a|^2 n + \bar{a}b + a\bar{b}) + 1 = 1\,,$$

  the term in the parentheses is zero, since the term by $J$ in eq. (3) must be zero.

- **$\delta$-coupling**
  It is a special case of permutation symmetric coupling, with the conditions

  $$\begin{aligned} f(\mathcal{X}) &\equiv f_i(\mathcal{X}) = f_j(\mathcal{X})\,, \quad \text{for all } i,j \in \{1,\dots,n\} \\ \sum_{j=1}^{n} f'_j(\mathcal{X}) &= \alpha f(\mathcal{X})\,. \end{aligned}$$

  The unitary matrix is $U = \frac{2}{n+i\alpha}J - I$.

- **standard (Kirchhoff, free, Neumann) conditions**
  This condition is the special kind of $\delta$-condition for $\alpha = 0$, i.e. functional value is continuous in the vertex and sum of outgoing derivatives is equal to 0. It is the most physical one, since the particle moves freely through the vertex. The name Kirchhoff is not a good choice since for all selfadjoint coupling conditions the probability current is conserved. The unitary matrix is $U = \frac{2}{n}J - I$.

- **Dirichlet conditions**
  In this case all functional values are zero. The unitary matrix is $U = -I$.

- **Neumann conditions**
  For this condition all the derivatives are zero. The unitary matrix is $U = I$.

# 4 Resolvent resonances and external complex scaling

In the current and following section we are interested in defining the resonances properly. By a resonance we understand a complex number. The physical meaning of this number is following. If the resonance is close to the real axis, the particle sent with the energy corresponding to its real part stays in the central part of the graph longer than for other energies. Its life time is longer, the closer the resonance to the real axis is. There are two main definitions of resonances, resolvent resonances and scattering resonances. Resolvent resonances are poles of the meromorphic continuation of the resolvent $(H - \lambda \mathrm{id})^{-1}$, where id is identity operator. The scattering resonances are poles of the continuation of the scattering matrix. It is more convenient to study the whole problem in the $k$-plane, where $k^2 = E$.

**Definition 4.1.** *There is a resolvent resonance at $k$ if there is a pole of the meromorphic continuation of the resolvent $(H - k^2\mathrm{id})^{-1}$. For the operator described in section 2 one can define a resolvent resonance as such $k$, for which there exists solution with the asymptotics $\alpha_j \mathrm{e}^{ikx}$ for all halflines.*

**Theorem 4.2.** *There are resolvent resonances only for $\operatorname{Im} k \leq 0$ or for $\operatorname{Re} k = 0$ (see figure 2).*

*Proof.* We know that the wavefunction components on the halflines are $g_j(x) = \alpha_j \mathrm{e}^{ikx}$. Let there be a resolvent resonance for $k = k_\mathrm{r} + ik_\mathrm{i}$ with $k_\mathrm{i} > 0$. Then there exists a solution of the Schrödinger equation on the graph with the above behaviour on the halflines. But the function $g_j(x) = \alpha_j \mathrm{e}^{ik_\mathrm{r}x}\mathrm{e}^{-k_\mathrm{i}x}$ is square integrable $\int_0^\infty |g_j(x)|^2 \,\mathrm{d}x < \infty$ and this means that $k^2$ is an eigenvalue of the Hamiltonian $H$. This contradicts the fact that the Hamiltonian is selfadjoint, since a selfadjoint Hamiltonian has only real eigenvalues (which corresponds to real or purely imaginary $k$). □

Resolvent resonances can be effectively studied by the method developed in 1970's by Aguilar, Baslev and Combes [AC71, BC71] called *external complex scaling*. The idea is to perform the transformation

$$U_\theta g(x) = \mathrm{e}^{\theta/2} g(\mathrm{e}^\theta x)\,.$$

on the external edges, while the internal edges are not scaled. For real $\theta$ this transformation is unitary, but it has the desired behaviour for $\theta$ with nontrivial imaginary part. We transform the Hamiltonian $H$ to a nonselfadjoint one

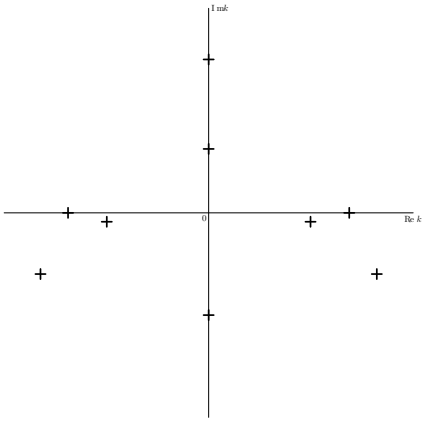


Figure 2: Resolvent resonances are only in the lower halfplane or on the imaginary axis

and then prove that resolvent resonance are eigenvalues of this nonselfadjoint operator.

**Theorem 4.3.** *Let $H_\theta = U_\theta H U_{-\theta}$ and $f_j$ be the wavefunction components on the internal edges, $g_j$ wavefunction components on the external edges. Then it acts as*

$$H_\theta \begin{pmatrix} f_j(x) \\ g_j(x) \end{pmatrix} = U_\theta H U_{-\theta} \begin{pmatrix} f_j(x) \\ g_j(x) \end{pmatrix} = \begin{pmatrix} -f_j''(x) + V_j(x) f_j(x) \\ -\mathrm{e}^{-2\theta x} g_j''(x) \end{pmatrix}$$

*Proof.* Clearly, the internal edges are not scaled, for the external edges we obtain

$$\begin{aligned} U_\theta(-\mathrm{d}^2/\mathrm{d}x^2)U_{-\theta} g_{j\theta}(x) &= U_\theta(-\mathrm{d}^2/\mathrm{d}x^2)\mathrm{e}^{-\theta/2} g_{j\theta}(-\mathrm{e}^\theta x) = \\ &= U_\theta \mathrm{e}^{-2\theta}\mathrm{e}^{-\theta/2} g_{j\theta}''(-\mathrm{e}^\theta x) = \mathrm{e}^{-2\theta}\mathrm{e}^{-\theta/2}\mathrm{e}^{-2\theta} g_{j\theta}''(x) = \mathrm{e}^{-2\theta} g_{j\theta}''(x)\,. \end{aligned}$$

□

Now we state a theorem on the spectrum of the scaled operator. The main idea of the external complex scaling is to obtain resonances as eigenvalues of this non-selfadjoint operator. The spectrum $\sigma(T)$ of the operator $T$ can be divided into two parts – *discrete spectrum* and *essential spectrum*. The discrete spectrum $\sigma_{\mathrm{d}}(T)$ is the set of eigenvalues with finite multiplicity which are isolated points of $\sigma(T)$; the essential spectrum is its complement in $\sigma(T)$. We will show the idea of the proof of the essential spectrum of the operator $H_\theta$ and complete proof of the fact that resolvent resonances are for imaginary part of $\theta$ large enough eigenvalues of $H_\theta$.

**Theorem 4.4.** *The essential spectrum of $H_\theta$ is $\mathrm{e}^{-2\theta}[0,\infty)$. The resonances of $H$ can be obtained as eigenvalues of $H_\theta$ for $\operatorname{Im}\theta$ large enough.*

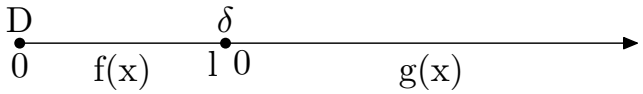


Figure 3: Example: a halfline with an appendix

*Proof.* Let $H_{\mathrm{D}\theta}$ be operator acting as $H_\theta$ with the coupling conditions changed to Dirichlet. Using Krein formula (which states that two selfadjoint extension of the same operator differ only by a compact operator) and Weyl's theorem (which states that if two operators differ by a compact operator, then their essential spectra are the same) one can prove that essential spectra of operators $H_{\mathrm{D}\theta}$ and $H_\theta$ are the same. Since the essential spectrum of minus second derivative on the halfline with Dirichlet coupling is $[0,\infty)$, the essential spectrum of the operator $H_{\mathrm{D}\theta}$ and hence $H_\theta$ is $\mathrm{e}^{-2\theta}[0,\infty)$.

Let $k^2$ with $k = k_\mathrm{r} + ik_\mathrm{i}$ be a resolvent resonance with $k_\mathrm{i} < 0$. Then the corresponding solution of the Schrödinger equation with the Hamiltonian $H$ has halfline components not square integrable. Let for simplicity be $\theta = i\vartheta$, $\vartheta \in \mathbb{R}$ and large enough $-\vartheta < \arg k < 0$. The component on the $j$-th edge is $g_{j\theta}(x) = \alpha_j \mathrm{e}^{i\vartheta/2}\exp(ik\mathrm{e}^{i\vartheta}x)$. Since $-\vartheta < \arg k$, is $\mathrm{Im}\,(k\mathrm{e}^{i\vartheta}) > 0$ and therefore $g_{j\theta}(x)$ is square integrable. Therefore, the solutions of the Schrödinger equation for $H$ are after the scaling the eigenvalues of $H_\theta$. □

Now we show an example, which shows how to compute resolvent resonances for a simple graph.

**Example 4.5.** *(a line with an appendix – resolvent resonances)*
*Let us consider a graph consisting of an abscissa of length $l$ and a halfline (see figure 3). There is a Dirichlet coupling at one end of the abscissa and $\delta$-coupling of strength $\alpha$ between the abscissa and the halfline. We assume the potential on the abscissa and the halfline to be zero. We parametrize the abscissa by the interval $(0,l)$ and the halfline by $(0,\infty)$ and describe the wavefunction components by $f$ and $g$, respectively. The coupling conditions can be written as*

$$f(0) = 0\,, \quad f(l) = g(0)\,, \quad -f'(l) + g'(0) = \alpha g(0)\,.$$

*We take a general ansatz for solutions of the Schrödinger equation as*

$$f(x) = a\mathrm{e}^{-ikx} + b\mathrm{e}^{ikx}\,, \quad g(x) = c\mathrm{e}^{-ikx} + d\mathrm{e}^{ikx}\,.$$

*Now we perform the scaling transformation $g_\theta(x) = U_\theta g(x) = \mathrm{e}^{\theta/2} g(\mathrm{e}^\theta x)$ with $\mathrm{Im}\,\theta > 0$ large enough and search for eigenvalues of operator $H_\theta$. Hence one can take $c = 0$ since the scaled function $c\mathrm{e}^{\theta/2}\mathrm{e}^{-ikx\mathrm{e}^\theta}$ is not square integrable. We have*

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

*The coupling conditions can be rewritten as*

$$\begin{aligned} a + b = 0\,, \quad a\mathrm{e}^{-ikl} + b\mathrm{e}^{ikl} &= \mathrm{e}^{-\theta/2} g_\theta(0)\,, \\ ik(a\mathrm{e}^{-ikl} - b\mathrm{e}^{ikl}) &= (\alpha - ik)\,\mathrm{e}^{-\theta/2} g_\theta(0)\,. \end{aligned}$$

*Using $b = -a$ we have*

$$a(\mathrm{e}^{-ikl} - \mathrm{e}^{ikl}) = \mathrm{e}^{-\theta/2} g_\theta(0)\,,$$
$$ika(\mathrm{e}^{-ikl} + \mathrm{e}^{ikl}) = (\alpha - ik)\,\mathrm{e}^{-\theta/2} g_\theta(0)\,.$$

*Now substituting from the first equation for $\mathrm{e}^{-\theta/2} g_\theta(0)$ to the second one and dividing the second equation by $(-2i)$ we obtain*

$$-ak\frac{\mathrm{e}^{ikl} + \mathrm{e}^{-ikl}}{2} = (\alpha - ik)a\frac{\mathrm{e}^{ikl} - \mathrm{e}^{-ikl}}{2i}$$

*which leads to the resonance condition*

$$(\alpha - ik)\sin kl + k\cos kl = 0\,.$$

# 5 Scattering resonances

The second possibility how to define resonances is as poles of the meromorphic continuation of the scattering matrix. In this view the compact part of the graph is a scattering center and the halflines are the leads. Since we consider zero potential on the halflines, the solution on the semiinfinite leads can be expressed as a linear combination of $\mathrm{e}^{-ikx}$ and $\mathrm{e}^{ikx}$. The first one we call the incoming wave and the second one the outgoing wave.

To elucidate why we have used this notation, let us for a while consider a time dependent Schrödinger equation on the halfline $(-\partial_x^2 - i\partial_t)u_j(x,t) = 0$. Its solution can be after separating the variables found in the form $u_j(x,t) = \mathrm{e}^{-itk^2} g_j(x)$, where $g_j(x)$ is the solution of time independent Schrödinger equation. Substituting the combination of $\mathrm{e}^{-ikx}$ and $\mathrm{e}^{ikx}$ we obtain $u_j(x) = c_j\mathrm{e}^{-ik(x+kt)} + d_j\mathrm{e}^{ik(x-kt)}$. The first wave is incoming (for growing $t$ the $x$ must be smaller to get the same exponent), the second one is outgoing.

The scattering matrix $S = S(k)$ is the operator, which maps the vector of amplitudes of the incoming waves into the vector of amplitudes of the outgoing waves. The complex energies, for which its entries diverge, are called scattering resonances.

**Example 5.1.** *Let us now study the same example as in the case of resolvent resonances. We again assume an abscissa of length $l$ and a halfline in figure 3 with Dirichlet coupling at one end of the segment and $\delta$-coupling between the abscissa and the halfline.*

$$f(0) = 0\,, \quad f(l) = g(0)\,, \quad -f'(l) + g'(0) = \alpha g(0)\,.$$

*We use the ansatz $f(x) = a\mathrm{e}^{-ikx} + b\mathrm{e}^{ikx}$ and $f(x) = c\mathrm{e}^{-ikx} + d\mathrm{e}^{ikx}$ and obtain*

$$a + b = 0\,, \quad a\mathrm{e}^{-ikl} + b\mathrm{e}^{ikl} = c + d\,,$$
$$ik(d - c) + ik(a\mathrm{e}^{-ikl} - b\mathrm{e}^{ikl}) = \alpha(c + d)\,.$$

*Substituting $b = -a$ we obtain*

$$a(\mathrm{e}^{-ikl} - \mathrm{e}^{ikl}) = c + d\,,$$
$$ik(d-c) + ika(\mathrm{e}^{-ikl} + \mathrm{e}^{ikl}) = \alpha(c+d)\,.$$

*Using definitions of sine and cosine and substituting now for $a$ from the first equation to the second we get*

$$ik(d-c)\sin kl - k\cos kl(c+d) = \alpha(c+d)\sin kl\,,$$
$$\left[(\alpha - ik)\sin kl + k\cos kl\right] d = -\left[(\alpha + ik)\sin kl + k\cos kl\right] c\,.$$

*We finally obtain*

$$S(k) = \frac{d}{c} = -\frac{(\alpha + ik)\sin kl + k\cos kl}{(\alpha - ik)\sin kl + k\cos kl}\,.$$

*The scattering matrix is in this case only a number (we have one halfline) and its poles give the same resonance condition as resolvent resonances.*

# 6 The equivalence of resonances

In this section we prove that for quantum graphs the two previous definitions of resonances are equivalent. To be precise, the set of resolvent resonances is equal to the set of scattering resonances unified with the set of eigenvalues with corresponding eigenfunctions supported on the internal part of the graph. This result was obtained first for certain set of coupling conditions in [EL07], for all graphs and hedgehog manifolds it was proved in [EL13].

**Theorem 6.1.** *Let us consider the quantum graph with the Hamiltonian defined in section 2. Then there is a resolvent resonance at $k_0^2$ iff there is a scattering resonance at $k_0^2$ or there is an eigenvalue at $k_0^2$ with the eigenfunction supported on the internal part of the graph.*

*Proof.* We assume the coupling condition 2 with $\Psi = \begin{pmatrix} \Psi_{\mathrm{int}} \\ \Psi_{\mathrm{ext}} \end{pmatrix}$ and $\Psi' = \begin{pmatrix} \Psi'_{\mathrm{int}} \\ \Psi'_{\mathrm{ext}} \end{pmatrix}$ Since the solution on the $j$-th internal edge is a combination of two linearly independent solutions $a_j u_j(x) + b_j v_j(x)$, we have entries of the vector of functional values $a_j u_j(v) + b_j v_j(v)$ ($v$ denotes the vertex), similarly for the vector of derivatives $a_j u'_j(v) + b_j v'_j(v)$. For an external edge we have solution as combination of incoming and outgoing wave $c_j \mathrm{e}^{-ikx} + d_j \mathrm{e}^{ikx}$, hence $\Psi_{\mathrm{ext}} = \mathbf{c} + \mathbf{d}$, $\Psi'_{\mathrm{ext}} = ik(\mathbf{d} - \mathbf{c})$.

Therefore, the coupling condition 2 can be rewritten as

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

where $A(k)$, $B(k)$ are $(2N+M)\times N$ energy-dependent matrices, $C(k)$, $D(k)$ are $(2N+M)\times M$ energy-dependent matrices and $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{d}$ are vectors with entries

$a_j$, $b_j$, $c_j$ and $d_j$. We define a $(2N+M)\times 2N$ matrix $E(k)=(A(k),B(k))$ and the vector $\mathbf{e}=\begin{pmatrix}\mathbf{a}\\ \mathbf{b}\end{pmatrix}$ corresponding to the internal coefficients. The previous equation can be thus rewritten as

$$E(k)\mathbf{e}+C(k)\mathbf{c}+D(k)\mathbf{d}=0\,. \tag{4}$$

If $E(k_0)$ has less then $2N$ linearly independent rows, it means that there exist a solution of (4) with $\mathbf{c}=\mathbf{d}=0$, i.e. eigenvalue with eigenfunction supported only on the internal part of the graph. We know that $k_0^2\in\mathbb{R}$. Clearly, this eigenvalue belongs also to the family of resolvent resonances (solutions with $\mathbf{c}=0$).

Now we assume that $E(k_0)$ has exactly $2N$ linearly independent rows. We rearrange the equations (4) so that first $2N$ rows of $E(k_0)$ are linearly independent. From these first $2N$ equations we express $\mathbf{e}$ and substitute it into the remaining $M$ equations. We obtain

$$\tilde{C}(k)\mathbf{c}+\tilde{D}(k)\mathbf{d}=0$$

with $M\times M$ matrices $\tilde{C}(k)$ and $\tilde{D}(k)$. The resolvent resonances are solutions with only outgoing waves, i.e. $\mathbf{c}=0$; this means that the resonance condition is $\det\tilde{D}(k)=0$. The scattering matrix is $S(k)=(\tilde{D}(k))^{-1}\tilde{C}(k)$, the condition for scattering resonances also is $\det\tilde{D}(k)=0$. Therefore these families of resonances coincide. □

# 7 Effective coupling on a finite graph

The content of this section will be used later. We will introduce effective coupling equation for the graph without halflines.

**Theorem 7.1.** *Let $H$ be a Schrödinger operator on a quantum graph $\Gamma$ with $2N$ internal and $M$ external edges and coupling given by $(2N+M)\times(2N+M)$ unitary matrix $U$ consisting of blocks*

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

*where the $2N\times 2N$ matrix $U_1$ corresponds to the coupling between internal edges, $M\times M$ matrix $U_4$ corresponds to the coupling between the halflines and $2N\times M$ matrix $U_2$ and $M\times 2N$ matrix $U_3$ correspond to the mixed coupling. Let $\{\lambda_i\}_{i=1}^M$ be eigenvalues of $U_4$. Then all resolvent resonances of $\Gamma$ with $k$ on $\mathbb{C}\backslash\{\frac{\lambda_1-1}{\lambda_1+1},\dots,\frac{\lambda_M-1}{\lambda_M+1}\}$ are given as eigenvalues of operator with the same action on the internal edges as $H$ but satisfying energy-dependent coupling conditions*

$$(\tilde{U}(k)-I_{2N})\vec{f}+i(\tilde{U}(k)+I_{2N})\vec{f}'=0$$

*with*

$$\tilde{U}(k)=U_1-(1-k)U_2[(1-k)U_4-(k+1)I_M]^{-1}U_3\,. \tag{5}$$

*Proof.* Let $\mathbf{f}$ and $\mathbf{g}$ denote the vector of amplitudes of functional values on the internal and external edges, respectively and let $\mathbf{f}'$ and $\mathbf{g}'$ be the vectors of amplitudes of outgoing derivatives. Then the coupling condition (2) can be rewritten as

$$\begin{pmatrix} U_1 - I_{2N} & U_2 \\ U_3 & U_4 - I_M \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix} + i \begin{pmatrix} U_1 + I_{2N} & U_2 \\ U_3 & U_4 + I_M \end{pmatrix} \begin{pmatrix} \mathbf{f}' \\ \mathbf{g}' \end{pmatrix} = 0\,,$$

where $I_N$ denotes the $N \times N$ unit matrix. Performing external complex scaling means replacing $\mathbf{g}$ and $\mathbf{g}'$ by $\mathrm{e}^{-\theta/2}\mathbf{g}_\theta$ and $ik\mathrm{e}^{-\theta/2}\mathbf{g}_\theta$, respectively.

$$\begin{pmatrix} U_1 - I_{2N} & U_2 \\ U_3 & U_4 - I_M \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \mathrm{e}^{-\theta/2}\mathbf{g}_\theta \end{pmatrix} + i \begin{pmatrix} i(U_1 + I_{2N}) & -kU_2 \\ iU_3 & -k(U_4 + I_M) \end{pmatrix} \begin{pmatrix} \mathbf{f}' \\ \mathrm{e}^{-\theta/2}\mathbf{g}_\theta \end{pmatrix} = 0\,.$$

Now eliminating $\mathbf{g}_\theta$ for $\det\left((1-k)U_4 - (k+1)I_M\right) \neq 0$ we get

$$\begin{aligned}[U_1 - I_{2N} - (1-k)U_2[(1-k)U_4 - (k+1)I_M]^{-1}U_3]\mathbf{f} + \\ + [U_1 + I_{2N} - (1-k)U_2[(1-k)U_4 - (k+1)I_M]^{-1}U_3]\mathbf{f}' = 0\end{aligned}$$

which can be written as

$$(\tilde{U}(k) - I_{2N})\mathbf{f} + i(\tilde{U}(k) + I_{2N})\mathbf{f}' = 0$$

with

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

We can easily show that the condition $\det\left((1-k)U_4 - (k+1)I_M\right) = 0$ which for eigenvalues means $(1-k)\lambda_j - (k+1) = 0$ implies $k = \frac{\lambda_j - 1}{\lambda_j + 1}$. With exception of these points the construction works. □

# 8 Asymptotics of resonances for non-magnetic graphs

We start the main part of this text by a topic which if at the first sight different from quantum graphs and their resonance properties. Asymptotical behaviour of the number of eigenvalues of Laplace-Beltrami operator on a Riemannian manifold of the dimension $d$ is given by Weyl's law [Wey11]. We show the result of Ivrii from [Ivr80]. The number of eigenvalues which are in modulus smaller than $\lambda$ is given by

$$N(\lambda) = \frac{\omega_d |\Omega|}{(2\pi)^d}\lambda^{d/2} \pm \frac{\omega_{d-1}|\partial\Omega|}{4(2\pi)^{d-1}}\lambda^{(d-1)/2} + o(\lambda^{(d-1)/2})\,,$$

where $\omega_d$ stands for the volume of a $d$-dimensional ball with radius 1 and $|\Omega|$ and $|\partial\Omega|$ denote the volume of the manifold and volume of its boundary, respectively.

The plus sign corresponds to the Neumann condition on the boundary of the manifold, the minus sign to the Dirichlet condition.

Now we will get the expression for the asymptotics of the number of eigenvalues of a compact quantum graph. We will work in the $k$-plane, where $k$ is the square root of energy. The formula for the number of eigenvalues in modulus smaller than $R$ is

$$N(R) = \frac{2V}{\pi} R + \mathcal{O}(1)\,, \tag{6}$$

where $V$ is the sum of the lengths of the (internal) edges. This result follows from the previous equation taking $\lambda = R^2$ and adding an extra factor of 2, because we count every eigenvalue twice since $(-k)^2 = k^2$.

Our aim will be to find the asymptotical behaviour of the number of resolvent resonances for a noncompact quantum graph. To be precise, we want the number of resolvent resonances enclosed in the circle of radius $R$ in the $k$-plane in the limit $R \to \infty$. We would expect that it behaves as the equation (6) with $V$ being the sum of the lengths of the internal edges of the graph. It holds true for most of the graphs (we will call these graphs *Weyl*), but there is a class of graphs for which the constant in the asymptotics is smaller than expected (we denote these graphs as *non-Weyl*).

The behaviour of the counting function of resolvent resonances was studied first for quantum graphs with standard condition by Davies and Pushnitski [DP11]. They found a nice geometric condition: the graph is non-Weyl iff it has a *balanced* vertex. By a balanced vertex we mean the vertex which connects the same number of internal and external edges. Later we generalized this result to all possible couplings in [DEL10]. We found a condition on the eigenvalues of the effective coupling matrix in the previous section which distinguishes the Weyl and non-Weyl graphs. In this text both results will be stated in the opposite order. First, we prove the theorem on the general graphs and then we show the condition by Davies and Pushnitski as its corollary.

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