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DOCTORAL THESIS



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Quantum Graphs and Their Generalizations

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To my parents.

I would like to thank professor Pavel Exner for numerous pieces of advice and invaluable help during writing the theses. I am also indebted to professor E. Brian Davies and dr. Rupert Frank for their pieces of advice.

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Název práce: Kvantové grafy a jejich zobecnění

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Abstrakt: V předkládané práci studujeme spektrální a rezonanční vlastnosti kvantových grafů. Nejdříve uvažujeme grafy, délky jejichž některých hran jsou soudělné. V konkrétních případech studujeme trajektorie rezonancí, které vzniknou porušením poměru délek hran. Dokážeme, že počet rezonancí se při této perturbaci lokálně zachovává. Hlavní část práce se zabývá asymptotikou počtu rezonancí. Najdeme kritérium, jak rozlišit grafy s neweylovskou asymptotikou (konstanta u vedoucího členu je nižší, než se očekává). Navíc vysvětlíme toto neweylovské chování konstrukcí unitárně ekvivalentního grafu. Pokud umístíme graf do magnetického pole, jeho základní charakteristika (weylovskost/neweylovskost) se nezmění. Může se ale změnit “efektivní velikost” neweylovského grafu. V poslední části práce popíšeme ekvivalenci mezi radiálními stromovými grafy a množinou hamiltoniánů na polopřímkách. Tento výsledek využijeme pro důkaz absence absolutně spojitého spektra pro širokou třídu řídkých stromových grafů.

Klíčová slova: kvantové grafy, Schrödingerovy operátory, rezonance, Weylův zákon

Title: Quantum Graphs and Their Generalizations

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Abstract: In the present theses we study spectral and resonance properties of quantum graphs. First, we consider graphs with rationally related lengths of the edges. In particular examples we study trajectories of resonances which arise if the ratio of the lengths of the edges is perturbed. We prove that the number of resonances under this perturbation is locally conserved. The main part is devoted to asymptotics of the number of resonances. We find a criterion how to distinguish graphs with non-Weyl asymptotics (i.e. constant in the leading term is smaller than expected). Furthermore, due to explicit construction of unitary equivalent operators we explain the non-Weyl behaviour. If the graph is placed into a magnetic field, the Weyl/non-Weyl characteristic of asymptotical behaviour does not change. On the other hand, one can turn a non-Weyl graph into another non-Weyl graph with different “effective size”. In the final part of the theses, we describe equivalence between radial tree graphs and the set of halfline Hamiltonians and use this result for proving the absence of the absolutely continuous spectra for a class of sparse tree graphs.

Keywords: quantum graphs, Schrödinger operators, resonances, Weyl’s law

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Introduction

Quantum graphs are a widely studied model which, despite its simplicity, can describe nontrivial effects and has a lot of application mainly in mesoscopic physics. An idea to replace a real physical system by a one-dimensional model is very old and can be traced back to works of Pauling [Pau36] from 1936, where diamagnetic properties of aromatic molecules were studied, and Ruedenberg and Scherr [RS53] from 1953, where such a model is worked out as a description of π -electrons in aromatic hydrocarbons. Nevertheless, intensive development of quantum graphs came in the last two decades only.

The model can be understood as a limit of *quantum wires* where the width of the wire is neglected. From the works on approximating Schrödinger operators on wires by a quantum graph we refer e.g. to [EP09]. Another possibility how to approach the model of quantum graphs is so called *leaky graph* (see e.g. [Exn07]) where a tunneling between nearby edges can be present.

A simple method how to measure spectral and resonance properties of quantum graphs have been presented by Hul at all [HBP⁺04]. Quantum graphs were simulated by a microwave network using optical cables.

Since from mathematical point of view this model is quite simple (a set of ordinary differential equations), quantum graphs can be used as a toy model of many systems. Attempts to understand quantum chaos on graphs have first been made by Kottos and Smilanski [KS97] who found connection between spectral statistics on graphs and random matrix theory. Furthermore, we can mention e.g. paper by Berkolaiko, Bogomolny and Keating [BBK01], where a star graph statistics is compared with a two-dimensional chaotical model – the so-called Šeba billiard.

For more information about various directions in quantum graphs and connected problems we refer to the proceedings [EKK⁺07].

In the present thesis we focus on spectral and especially resonance properties of quantum graphs. In the first chapter, an introduction to the whole model is given and coupling conditions at the vertices of the graph are studied. The second chapter focuses on the spectrum of quantum graphs and properties of resonances. Resolvent and scattering resonances are introduced and introduction to the Weyl's asymptotics is given. The third chapter tries to summarize the results of the theses, while the original articles on which the theses is based are attached in appendices.

Appendix A deals with resonances which arise from eigenvalues of the graph if

the lengths of the edges of the graph are perturbed. If a graph has commensurate lengths of some of its edges and a suitable coupling is applied, eigenfunctions with zeros at the vertices of the graph can be found. Hence eigenvalues embedded into the continuous spectrum may be present. If this rationality is violated, some of the eigenvalues may become resonances. First, we describe a general approach how to obtain a resonance condition. Then we give two theorems stating the conditions on the coupling under which certain eigenvalues are present. Furthermore, we prove that the number of resolvent resonances with multiplicities taken into account is locally conserved. In the end of this article we also add two particular examples with explicit trajectories of resonances depending on the length parameter which were obtained in [Lip08].

In the paper in appendix B the resonance asymptotics is studied. We generalize the results of Davies and Pushnitski obtained for Kirchhoff's coupling and we give a condition which distinguishes expected Weyl behaviour from the non-Weyl one. Furthermore, we introduce a construction which elucidates why there are less resonances in the non-Weyl case than expected. We also study asymptotical behaviour of weighted graphs. Finally, we give arguments why it is difficult to generally determine the "effective size" of a graph, since this issue is a global characteristic of the graph.

The third appendix deals with resonance asymptotics of magnetic quantum graphs. Two main results are obtained. Firstly, placing a graph into a magnetic field does not change the Weyl asymptotics into a non-Weyl one and vice versa. However, for a graph which is already non-Weyl the magnetic field can change its "effective size" (the constant in the leading term of asymptotics).

In appendix D the conditions under which a tree graph does not have absolutely continuous spectrum are studied. The unitary equivalence between operator on a radial tree graph and orthogonal sum of operators on the halflines is established for a large class of coupling conditions. This generalized the result by Sobolev and Solomyak [SS02] and a construction in [Lip08]. In the second part of the paper, this equivalence is used for proving that (under some conditions on the coupling parameters) sparse tree graphs do not possess absolutely continuous spectrum. On the other hand, examples where this does not hold true are given.

Chapter 1

Schrödinger operators on graphs

1.1 Description of the model

We start by introducing the model of quantum graphs and stating basic definitions. For simplicity, we assume that the graph has finitely many edges; the extension to graphs with infinitely many edges and to operators on manifolds is straightforward and is given in following chapters.

The main setting of our model is a metric graph equipped with a second order differential operator. By Γ we denote a metric graph which consists of the set of vertices $\mathcal{V} = \{\mathcal{X}_j\}$, the set of internal edges \mathcal{E}_i and external edges \mathcal{E}_e . The internal edges connect two vertices from \mathcal{V} and a positive length l_i is assigned to each of them. The external leads are equivalent to halflines $[0, \infty)$ and provide a setting to study scattering.

Let us suppose that quantum graph Γ has N internal and M external edges. The Hilbert space we work in consists of functions square integrable on all edges

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

Its entries are described by columns

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

The first word in “quantum graphs” is represented by the quantum Hamiltonian, which acts as $-d^2/dx^2 + V(x)$ on the internal edges and as $-d^2/dx^2$ on the external ones. For the sake of simplicity, we assume the choice of units $\hbar = 1, m = 1/2$, in which the constant before the second derivative is -1 . The potential on the internal edges $V(x)$ is a real bounded function, continuous at each vertex. The domain of the Hamiltonian consists of functions in the Sobolev space $W^{2,2}(\Gamma)$ (orthogonal sum of Sobolev spaces on each edge) which fulfill the vertex coupling conditions described below.

At each vertex \mathcal{X}_j suitable coupling conditions are imposed. They connect the vector of limits of functional values from each edge

$$\Psi_j = (\psi_{j1}(\mathcal{X}_j), \dots, \psi_{jn_j}(\mathcal{X}_j))^T$$

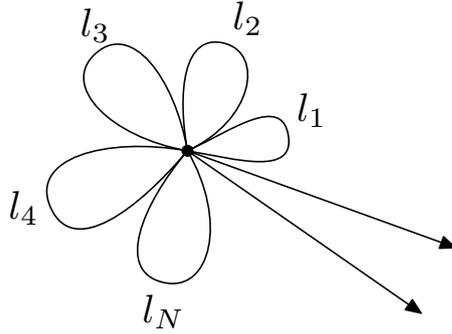


Figure 1.1: A flower-like graph

with the vector of limits of outgoing derivatives

$$\Psi'_j = (\psi'_{j1}(\mathcal{X}_j), \dots, \psi'_{jn}(\mathcal{X}_j))^T.$$

Here $\psi_{ji}(x)$ is a wavefunction on a i -th edge emanating from \mathcal{X}_j , similarly $\psi'_{ji}(x)$ is its derivative taken in the direction away from the vertex and n is the degree of the vertex \mathcal{X}_j (the number of edges, both internal and external, which emanate from it). Then the general coupling condition describing a selfadjoint operator is for each vertex \mathcal{X}_j given by

$$(U_j - I_n)\Psi_j + i(U_j + I_n)\Psi'_j = 0. \quad (1.1)$$

where U_j is a unitary $n \times n$ matrix and I_n stands for unit matrix of the same size.

Finding the point spectrum of this Hamiltonian means solving time-independent Schrödinger equation $H\psi = k^2\psi$ which decouples into several differential equations.

1.2 The flower-like graph description

We introduce a model with only one vertex, which is more suitable for proving claims for general graphs. The trick ([Kuc05, Kuc08]) is very simple; one joins all the vertices together (see figure 1.1) and describes the coupling on the whole graph by one big unitary matrix U . This matrix not only describes the coupling but also encodes the structure of the graph. It is easy to see that if one chooses U as block-diagonal, the coupling conditions decouple into the conditions for separate vertices (1.1).

Theorem 1.2.1. *(every graph is a flower)*

Let Γ_1 be a quantum graph consisting of the set of vertices $\{\mathcal{X}_j\}_{j=1}^s$, N internal edges of lengths l_1, \dots, l_N and M external edges. Let $H_1 = -d^2/dx^2 + V(x)$ be the Hamiltonian defined in the previous section with the coupling at the vertices of Γ_1 given by matrices U_j and conditions (1.1). Let Γ_2 be a graph with only one

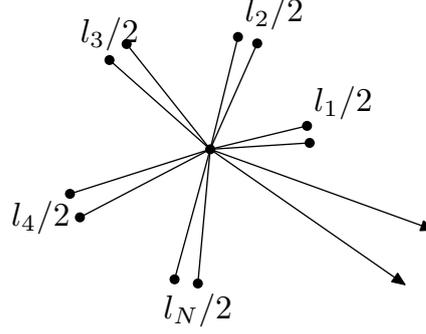


Figure 1.2: A star graph corresponding to the flower-like graph

vertex which joins N internal edges of lengths l_1, \dots, l_N and M external edges. By H_2 we denote a Hamiltonian which acts in the same way as H_1 with the same potential on the corresponding edges and with the coupling

$$(U - I)\Psi + i(U + I)\Psi' = 0 \quad (1.2)$$

where $U = \text{diag}(U_1, U_2, \dots, U_s)$ is a $(2N + M) \times (2N + M)$ unitary matrix consisting of blocks U_j ; I stands for a unit matrix of the same size and $\Psi = (\Psi_1^T \dots, \Psi_s^T)^T$. Then H_1 is unitarily equivalent to H_2 .

Proof. It follows from the definition of the operator H_2 that for each edge one obtains the same differential equation. Due to the block diagonality of U the coupling condition (1.2) splits to the system (1.1). \square

When dealing with the matrix U it is more convenient to rearrange its columns and corresponding entries of Ψ and Ψ' in the way that the last M entries of Ψ and Ψ' correspond to the external edges and first $2N$ are arranged in pairs – beginning and end of the given edge. From now on we suppose that such a rearrangement has already been done. This model significantly reduces the number of technicalities for a general graph and we will use it in the following sections and chapters.

For the sake of completeness we give a theorem which states that every quantum graph with a finite number of edges can be, similarly to the flower-like model, regarded also as a star graph.

Theorem 1.2.2. (every graph with symmetric potential is a star)

Let Γ_2 be a flower-like graph and H_2 be the Hamiltonian defined in theorem 1.2.1 with coupling given by matrix U . We denote by $V_r(x)$ the potential on the r -th edge and suppose that $V_r(x) = V_r(l_r - x)$. Let Γ_3 be a star graph (see figure 1.2) connecting $2N$ internal edges and M external edges. The internal edges are arranged in pairs; each edge of the r -th pair of them has length $l_r/2$. We denote by H_3 the Hamiltonian on Γ_3 acting as $-\text{d}^2/\text{d}x^2$ on the first edge of the r -th pair and as $-\text{d}^2/\text{d}x^2 + V_r(x)$ on the second one. We impose Dirichlet coupling condition ($f(l_r/2) = 0$) at the loose end of the first edge of each pair and Neumann

condition ($f'(l_r/2) = 0$) at the loose end of the second one. The coupling conditions at the central vertex of the star is given by equation (1.2) with U replaced by $W^{-1}UW$ where W is a block diagonal matrix consisting of blocks $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ for the subspace corresponding to previously described pairs of internal edges and a unit matrix for the subspace corresponding to the external edges.

Proof. We start with a previously introduced flower-like graph consisting of N internal and M external edges and construct a unitary equivalent star graph. First, we introduce a vertex in the middle of each loop and impose a Kirchhoff coupling condition (continuity of functional values and first derivatives). Let $f_r(x) \in W^{2,2}((0, l_r))$ be a projection to the r -th edge of an element of $D(H_2)$. Then we define $f_{r,\text{sym}}(x), f_{r,\text{ant}}(x) \in W^{2,2}((0, l_r))$ by

$$\begin{aligned} f_{r,\text{sym}}(x) &= \frac{1}{\sqrt{2}}(f_r(x) + f_r(l_r - x)) \\ f_{r,\text{ant}}(x) &= \frac{1}{\sqrt{2}}(f_r(x) - f_r(l_r - x)) \end{aligned}$$

One can straightforwardly check that both symmetric and antisymmetric part of f_r satisfy

$$\left(-\frac{d^2}{dx^2} + V_r(x)\right) f_{r,\text{sym}}(x) = 0, \quad -\frac{d^2}{dx^2} f_{r,\text{ant}}(x) = 0.$$

From the continuity of $f_r(x)$ and $f'_r(x)$ at $x = l_r/2$ we obtain Dirichlet and Neumann condition for $f_{r,\text{ant}}$ and $f_{r,\text{sym}}$, respectively. Similarly, the coupling conditions at the central vertex must be changed by a unitary transformation given by matrix W . \square

1.3 Schrödinger operators on graphs as selfadjoint extensions of a symmetric operator

In this section we give justification of the coupling condition (1.1) – following the results of Kostykin and Schrader [KS99, KS00] and Harmer [Har00]. We prove that the mentioned condition uniquely describes all selfadjoint Hamiltonians on the graph. We use the results of von Neumann's extension theory and the theory of Hermitian symplectic spaces to construct selfadjoint extensions.

First, we recall relevant propositions from the extension theory and sketch their proofs. More details could be found e.g. in textbooks [BEH08, RS75].

Definition 1.3.1. *Let L be an operator in the Hilbert space \mathcal{H} with scalar product (\cdot, \cdot) . We denote by L^* its adjoint, the operator acting as $L^*y = y^*$ with $(y, Lx) = (y^*, x)$ for all $x \in D(L)$. Its domain consists of all y for which the above relation holds true. The operator L is called symmetric if $(y, Lx) = (Ly, x)$ and selfadjoint if $L = L^*$, i.e. not only L is symmetric but also domains of L and L^* coincide. A selfadjoint operator L_1 is called a selfadjoint extension of a symmetric operator L if $D(L) \subset D(L_1)$ and $L = L_1$ on $D(L)$.*

Theorem 1.3.2. *Let L be a closed symmetric operator and L^* its adjoint. Then $\dim(\text{Ker}(\lambda \text{Id} - L^*))$ is constant for all λ with $\text{Im } \lambda > 0$ and all λ with $\text{Im } \lambda < 0$.*

Proof. From now on, we omit for simplicity the identity operator Id when possible. It suffices to prove that dimension of the kernel of $(\lambda - L^*)$ is locally constant. Without loss of generality we choose λ_1, λ_2 with $\text{Im } \lambda_1 > 0$ and $\text{Im } \lambda_2 > 0$ close to each other $|\lambda_2 - \lambda_1| < |\text{Im } \lambda_2|$. Let us suppose that the theorem does not hold, i.e. there exists such a $u \in \text{Ker}(\lambda_1 - L^*) \cap \text{Ker}(\lambda_2 - L^*)^\perp$ and $\|u\| = 1$. Then

$$u \in \text{Ker}(\lambda_2 - L^*)^\perp = \text{Ran}(\bar{\lambda}_2 - L) \quad \Rightarrow \quad \exists \varphi : u = (\bar{\lambda}_2 - L)\varphi.$$

$$\begin{aligned} u \in \text{Ker}(\lambda_1 - L^*) \quad \Rightarrow \quad 0 &= ((\lambda_1 - L^*)u, \varphi) = (u, (\bar{\lambda}_1 - L)\varphi) = \\ &= (u, (\bar{\lambda}_1 - \bar{\lambda}_2)\varphi) + (u, (\bar{\lambda}_2 - L)\varphi) = \|u\|^2 + (\bar{\lambda}_1 - \bar{\lambda}_2)(u, \varphi). \end{aligned} \quad (1.3)$$

On the other hand, from the symmetricity of L we have

$$\|u\|^2 = \|(\bar{\lambda}_2 - L)\varphi\|^2 = (\text{Im } \bar{\lambda}_2)^2 \|\varphi\|^2 + \|(\text{Re } \bar{\lambda}_2 - L)\varphi\|^2 \geq (\text{Im } \bar{\lambda}_2)^2 \|\varphi\|^2$$

and by

$$|(\bar{\lambda}_1 - \bar{\lambda}_2)(u, \varphi)| \leq \frac{|\bar{\lambda}_1 - \bar{\lambda}_2| \|u\|^2}{|\text{Im } \lambda_2|} < \|u\|^2.$$

we come to a contradiction with (1.3). \square

Hence, one can choose $\lambda = \pm i$ to describe dimensions of kernels of $(\lambda - L^*)$ in the upper and lower halfplane.

Definition 1.3.3. *Let L be a closed symmetric operator and L^* its adjoint. Then $\mathcal{N}_\pm \stackrel{\text{def}}{=} \text{Ker}(L^* \pm i)$ are called deficiency subspaces and their dimensions $n_\pm \stackrel{\text{def}}{=} \dim(\text{Ker}(L^* \pm i))$ are deficiency indices. The usual notation is (n_+, n_-) .*

Theorem 1.3.4. *(the first von Neumann's formula)*

Let L be a closed symmetric operator. One can uniquely decompose any $u \in D(L^)$ into $D(L)$, \mathcal{N}_+ and \mathcal{N}_- by*

$$u = u_0 + u_+ + u_-, \quad L^*u = Lu_0 - i(u_+ - u_-).$$

where $u_0 \in D(L)$, $u_\pm \in \mathcal{N}_\pm$.

Now we give our attention to selfadjoint extensions of Schrödinger operators on graphs. Let us consider a flower-like graph consisting of N internal and M external edges and construct all possible selfadjoint Hamiltonians in $L^2(\Gamma)$ acting as $-\text{d}^2/\text{d}x^2 + V_j(x)$. We start from a symmetric Hamiltonian H_0 with the domain consisting of functions in $W^{2,2}(\Gamma)$ satisfying the condition that both functional values and derivatives from each direction vanish at the central vertex. This operator has deficiency indices $(2N + M, 2N + M)$ and domain of its adjoint is $W^{2,2}(\Gamma)$ without any boundary conditions at the central vertex.

Selfadjoint extensions can be linked to the coupling conditions at the central vertex of the graph. A tool which is in this case more suitable than abstract von Neumann's theory is 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 write

$$\Omega(\phi, \psi) = \omega([\Phi], [\Psi]) = \bar{\Phi} \Psi' - \bar{\Phi}' \Psi = ([\Phi], \mathcal{J}[\Psi])_{\mathbb{C}^{4N+2M}}.$$

with $\mathcal{J} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ and vectors $[\Phi] = (\Phi, \Phi')^T$, $[\Psi] = (\Psi, \Psi')^T$. One can easily see that form $\Omega(\phi, \psi) = 0$ on the domain of H_0 and consequently also ω vanishes at corresponding subspace.

Definition 1.3.5. *Let W be a subspace of \mathbb{C}^{4N+2M} . We denote by $W^\perp = \{[\Psi] \in \mathbb{C}^{4N+2M} : ([\Psi], \omega[\Phi])_{\mathbb{C}^{4N+2M}} = 0, \forall [\Phi] \in W\}$. We call a subspace W of \mathbb{C}^{4N+2M} isotropic if $W^\perp \subset W$. We call it maximal isotropic or a Lagrangian plane if $W^\perp = W$.*

Our task is now to find all maximal isotropic subspaces of \mathbb{C}^{4N+2M} on which the form ω vanishes. It can be done by methods of symplectic Hermitian theory (see e.g. [Har00, KS99]), however, for the proof of the main theorem of this section we use a simple argument from [FT00] originally based on physical reasons.

Theorem 1.3.6. *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 (1.2).*

Proof. As stated before, we prove that all maximal isotropic subspaces are parametrized by equation (1.2). First we show that all subspaces parametrized by (1.2) are Lagrangian planes. Necessary condition for $\omega(\Phi, \Psi)$ to be zero for all Φ, Ψ in W is that $\omega(\Phi, \Phi) = 0$ for all $\Phi \in W$. We may notice that

$$0 = 2i\omega(\Phi, \Phi) = \|\Phi + i\Phi'\|^2 - \|\Phi - i\Phi'\|^2.$$

Hence vectors $\Phi + i\Phi'$ and $\Phi - i\Phi'$ have the same norm and must be related by a unitary matrix U . Equation (1.2) follows immediately.

Now we prove the opposite direction. We check by an explicit computation that every subspace parametrized by (1.2) is a Lagrangian plane. First, we notice that the form ω can be rewritten as

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

where V is a $(2N + M) \times (2N + M)$ unitary matrix. Using this fact and the equivalent form of the condition (1.2)

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

with D unitary and diagonal we need now only to check condition (1.2) for diagonal matrices. For D having no eigenvalues -1 we obtain $V\Psi' = i(D + I)^{-1}(D - I)V\Psi$, $(V\Phi')^* = (V\Phi)^*(-i)(D^* - I)(D^* + I)^{-1}$ 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 , in particular $(D + I)(D^* - I) + (D - I)(D^* + I) = 0$, the form vanishes for every $[\Phi]$, $[\Psi]$ fulfilling (1.2). If D has eigenvalues -1 , from the coupling condition follows that entries of $V\Psi$ and $V\Phi$ corresponding to these eigenvalues vanish. Hence the form $\omega(\Phi, \Psi)$ is equal to zero. \square

Remark 1.3.1. The condition $\omega(\Phi, \Phi) = \bar{\Phi}\Phi' - \bar{\Phi}'\Phi = 0$ has a simple physical interpretation. It means conservation of the probability current ($j = \frac{\hbar}{2mi}(\bar{\phi}\phi' - \phi\bar{\phi}')$) through the central vertex. In the proof we could have used the difference $\|\Phi + i\Phi'\|^2 - \|\Phi - i\Phi'\|^2$ with $l \in \mathbb{R}$ which would add l to the second term of (1.2). However, this does not add any additional degree of freedom since l can be related to U . The choice of l just fixes the length scale.

Remark 1.3.2. If one starts from a multiple vertex graph, constructs a flower-like graph and describes selfadjoint extension by the formula (1.2), one must take into account that also physically not very relevant Hamiltonians allowing the particle “hopping” between different vertices are included. We can easily get rid of it by requiring block diagonality of U in the basis which corresponds to actual topology of the graph.

1.4 Alternative descriptions of coupling conditions

However, there alternative descriptions of coupling conditions are for various reasons used in some articles. In this subsection we give a comparison of these descriptions, including their advantages and drawbacks.

We suppose that n edges emanate from a given vertex (for simplicity we omit the subscript referring to it).

- (Kostykin, Schrader [KS99])

The coupling between the vector of functional values and the vector of derivatives is given by two $n \times n$ square matrices A and B

$$A\Psi + B\Psi' = 0.$$

The Hamiltonian is selfadjoint iff the rectangular matrix (A, B) has maximal rank and $AB^* = BA^*$, where $*$ denotes adjoint (Hermitian conjugation) of the given matrix. The main disadvantage is nonuniqueness of this description (see theorem 1.4.1).

- (Kuchment [Kuc04, Kuc08])

Vaguely said, this alternative separates the Dirichlet, Neumann and Robin part of the coupling conditions. It uses mutually orthogonal projectors P , Q , and R . P and Q project to kernels $\text{Ker}(U + I)$ and $\text{Ker}(U - I)$, respectively, and $R = \text{Id} - P - Q$. The coupling can be expressed as follows.

$$P\Psi = 0, \quad Q\Psi' = 0, \quad R\Psi' = LR\Psi,$$

where operator L is selfadjoint. This coupling is useful namely for expressing the Hamiltonian in the language of quadratic forms.

- (Exner, Turek [ET07])

Let m be multiplicity of eigenvalue -1 of matrix U . Then the coupling can be expressed in ST -form

$$\begin{pmatrix} -S & 0 \\ -T^* & I_{n-m} \end{pmatrix} \Psi + \begin{pmatrix} I_m & T \\ 0 & 0 \end{pmatrix} \Psi' = 0.$$

with S selfadjoint $(n - m) \times (n - m)$ matrix, T being $(n - m) \times m$ matrix and I_s denoting $s \times s$ unit matrix. The described convention allows for explicit parametrization of the coupling and diminishes the number of parameters needed. Similarly to the previous description one can separate also eigenvalues $+1$ from the second subspace and write so called PQRS form. For more details see [CET10].

Finally, for reader's convenience, we give two theorems concerning relationships between different coupling matrices and the selfadjointness conditions for them.

Theorem 1.4.1. *(connection of different descriptions of couplings)*

The connection of the equivalent coupling described above to the coupling (1.1) is given by the following relations.

a)

$$A = C(U - I), \quad B = iC(U + I), \quad U = -(A + iB)^{-1}(A - iB),$$

where C is an arbitrary regular $n \times n$ matrix.

b) Let $U = V^{-1} \begin{pmatrix} -I_{m_1} & 0 & 0 \\ 0 & I_{m_2} & 0 \\ 0 & 0 & D \end{pmatrix} V$ with D being diagonal unitary matrix

which does not have eigenvalues -1 . Then projectors P , Q , R and the selfadjoint operator L can be represented by matrices

$$P = V^{-1} \begin{pmatrix} I_{m_1} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} V, \quad Q = V^{-1} \begin{pmatrix} 0 & 0 & 0 \\ 0 & I_{m_2} & 0 \\ 0 & 0 & 0 \end{pmatrix} V,$$

$$R = V^{-1} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I_{n-m_1-m_2} \end{pmatrix} V,$$

$$L = V^{-1} \begin{pmatrix} I_{m_1} & 0 & 0 \\ 0 & I_{m_2} & 0 \\ 0 & 0 & i(D + I_{n-m_1-m_2})^{-1}(D - I_{n-m_1-m_2}) \end{pmatrix} V.$$

The reverse relation is

$$U = -P + Q - R(L - iI)^{-1}(L + iI)R.$$

c)

$$U = -I_n + 2 \begin{pmatrix} I_m & 0 \\ T^* & 0 \end{pmatrix} \begin{pmatrix} (I_m + TT^* + iS)^{-1} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} I_m & T \\ 0 & 0 \end{pmatrix}.$$

Proof. a) The general relations for matrices A and B are obtained by multiplying the equation (1.1) by an arbitrary regular matrix C . From a linear combination of these two one obtains the expression for C . Substituting into a different linear combination we get the reverse relation representing U in terms of A and B .

b) The expressions can be straightforwardly checked.

c) The relation straightforwardly follows from a) using the fact that $U + I = -iC^{-1}B = 2i(A + iB)^{-1}B$.

□

Theorem 1.4.2. (*selfadjointness of the Hamiltonian*)

The Hamiltonian in representations a), b), c) is selfadjoint if following conditions are satisfied.

a) $AB^* = BA^*$ and $\text{rank}(A, B)$ is maximal.

b) L is selfadjoint

c) S is selfadjoint

Proof. Proof of a) and b) follows from the previous theorem and properties of unitary matrices. Proof of c) follows straightforwardly from a), condition for maximality of the rank is satisfied due to presence of unit matrices. □

1.5 Examples of coupling conditions

For the most used cases of coupling conditions we give a comparison of various descriptions. For simplicity, in the whole section we study the coupling at the vertex \mathcal{X} and suppose that there are n edges emanating from \mathcal{X} . In the following text J denotes $n \times n$ matrix with all entries equal to one and I is $n \times n$ identity matrix.

- permutation symmetric coupling

This type of coupling is not effected by perturbation of any two (or several) leads. The coupling matrix can be written in the form $U = aJ + bI$. Using relations $J^2 = nJ$ and $JI = IJ = J$ we obtain from unitarity of U that $|b|^2 = 1$ and $|na + b| = 1$.

- δ -conditions

$$f(\mathcal{X}) \equiv f_i(\mathcal{X}) = f_j(\mathcal{X}), \quad \text{for all } i, j \in \{1, \dots, n\}$$

$$\sum_{j=1}^n f'_j(\mathcal{X}) = \alpha f(\mathcal{X}).$$

One can rewrite this coupling into the language of A and B and by theorem 1.4.1 obtain also other coupling descriptions.

$$A = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ \alpha/n & \alpha/n & \alpha/n & \cdots & \alpha/n & \alpha/n \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{pmatrix}.$$

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

- δ'_s -conditions

The counterpart of δ condition which interchanges the role of the functional value and the derivative is called δ' condition. There are two generalizations of the coupling on the straight line to the vertex connecting n leads. The first one satisfies the permutation symmetry.

$$f'(\mathcal{X}) \equiv f'_i(\mathcal{X}) = f'_j(\mathcal{X}), \quad \text{for all } i, j \in \{1, \dots, n\}$$

$$\sum_{j=1}^n f_j(\mathcal{X}) = \beta f'(\mathcal{X}).$$

$$A = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ \beta/n & \beta/n & \beta/n & \cdots & \beta/n & \beta/n \end{pmatrix}.$$

$$U = I - \frac{2}{n - i\beta} J.$$

- δ' -conditions

The second generalization of δ' -condition reads as follows.

$$f_i(\mathcal{X}) - f_j(\mathcal{X}) = \frac{\beta}{n}(f'_i(\mathcal{X}) - f'_j(\mathcal{X})), \quad \text{for all } i, j \in \{1, \dots, n\}$$

$$\sum_{j=1}^n f'_j(\mathcal{X}) = 0.$$

$$A = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix},$$

$$B = \begin{pmatrix} -\beta/n & \beta/n & 0 & \cdots & 0 & 0 \\ 0 & -\beta/n & \beta/n & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -\beta/n & \beta/n \\ 1 & 1 & 1 & \cdots & 1 & 1 \end{pmatrix}.$$

$$U = \frac{2}{n - i\beta}J - \frac{n + i\beta}{n - i\beta}I.$$

- Kirchhoff's (free) conditions

These conditions are the most physical ones since the particle moves freely through the vertex. Sometimes also the term “Neumann” is used. In the view of remark 1.3.1 the name is better because the probability current conservation is satisfied for all selfadjoint couplings. Kirchhoff's coupling can be obtain as a special case of δ -conditions with the coupling strength equal to zero.

$$A = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{pmatrix}.$$

$$U = \frac{2}{n}J - I.$$

- Dirichlet conditions

This alternative separates all the edges in the vertex \mathcal{X} requiring that all functional values are zero.

$$A = I, \quad B = 0, \quad U = -I,$$

where 0 denotes matrix with all entries equal to zero.

- Neumann conditions

The counterpart of Dirichlet condition is Neumann coupling condition which requires vanishing of the derivatives from all directions.

$$A = 0, \quad B = I, \quad U = I.$$

Chapter 2

Spectral and resonance properties of quantum graphs

2.1 Spectrum of graphs with finitely many internal and external edges

In this section we revise basic spectral properties of quantum graphs with finitely many edges.

Definition 2.1.1. *Let T be an (in general unbounded) operator in the Hilbert space \mathcal{H} with the domain \mathcal{D} . Then by the resolvent set we call the set of all $\lambda \in \mathbb{C}$ for which the operator $T - \lambda I$ has a bounded inverse, i.e. there exist operator $R(\lambda)$ such that*

$$R(\lambda)(T - \lambda I) = I_{\mathcal{D}}, \quad (T - \lambda I)R(\lambda) = I_{\mathcal{H}}.$$

The operator $R(\lambda)$ we call the resolvent and we denote by $\rho(\lambda)$ the resolvent set. Its complement we call spectrum and denote by $\sigma(T)$. We can divide it into three classes:

- *point spectrum $\sigma_p(T)$: T is not injective, i.e. there exists such $x \in \mathcal{D}$ that $Tx = \lambda x$*
- *continuous spectrum $\sigma_c(T)$: $\text{Ran}(T - \lambda) \neq \mathcal{H}$, but it is dense in \mathcal{H}*
- *residual spectrum $\sigma_r(T)$: $\overline{\text{Ran}(T - \lambda)} \neq \mathcal{H}$*

Another division of spectra can be done as follows.

Definition 2.1.2. *Let T be an operator in the Hilbert space \mathcal{H} . Then its discrete spectrum $\sigma_d(T)$ is the set of eigenvalues with finite algebraic multiplicity which are isolated points $\sigma(T)$. The complement of the discrete spectrum is called essential spectrum and it is denoted by σ_{ess} .*

Definition 2.1.3. *Let us decompose the spectral measure by the Lebesgue's decomposition theorem into $\mu = \mu_{\text{ac}} + \mu_{\text{sc}} + \mu_{\text{pp}}$, where μ_{ac} is absolutely continuous part, μ_{sc} is singularly continuous part and μ_{pp} is pure point part (a discrete measure). By spectral theorem one can split the Hilbert space into parts $\mathcal{H} = \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}} \oplus \mathcal{H}_{\text{pp}}$. By restrictions of $\sigma(T)$ into these three subspaces we subsequently define absolutely continuous spectrum σ_{ac} , singularly continuous spectrum σ_{sc} and pure point spectrum σ_{pp} .*

We now give an alternative criterion how to find essential spectrum, for the proof we refer e.g. to [HS96]. Consequently, we use it to prove Weyl's theorem which states that compact perturbation does not change the essential spectrum.

Theorem 2.1.4. *(Weyl's criterion)*

Let A be a selfadjoint operator. Then $\lambda \in \sigma_{\text{ess}}$ iff there exist an orthonormal sequence $\{u_n\}_{n=1}^{\infty}$ such that $\|u_n\| = 1$, u_n weakly converges to 0 and $(A - \lambda)u_n$ strongly converges to 0 ($\|(A - \lambda)u_n\| \rightarrow 0$).

Theorem 2.1.5. *(Weyl's theorem)*

Suppose that A and B are selfadjoint operators in \mathcal{H} and $A - B$ is compact. Then $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$.

Proof. Suppose that $\sigma_{\text{ess}}(A) = 0$. Then there exists an orthonormal sequence u_n satisfying the conditions of Weyl's criterion. We know that u_n weakly converges to 0. Since $A - B$ is compact and a compact operator maps weakly converging sequences into norm convergent ones, we also have $\|(A - B)u_n\| \rightarrow 0$. Hence by triangle inequality

$$\|(B - \lambda I)u_n\| \leq \|(A - \lambda I)u_n\| + \|(B - A)u_n\| \rightarrow 0.$$

Hence we have $\sigma_{\text{ess}}(A) \subset \sigma_{\text{ess}}(B)$; the opposite inclusion is clear due to the symmetry. \square

We also give Krein's formula (see e.g. [AGHKH05]) which compares resolvents of two different selfadjoint extensions of a symmetric operator.

Theorem 2.1.6. *(Krein's formula)*

Let H_0 be a symmetric operator with deficiency indices (n, n) and H_1 and H_2 its selfadjoint extensions. Then

$$(H_1 - z)^{-1} = (H_2 - z)^{-1} + \sum_{i,j=1}^m \lambda_{ij}(z) (\psi_j(\bar{z}), \cdot) \psi_i(z), \quad z \in \rho(H_1) \subset \rho(H_2),$$

where

$$\psi_i(z) = \psi_i(z_0) + (z - z_0)(H_2 - z)^{-1} \psi_i(z_0), \quad i = 1, \dots, m$$

with $\psi_i(z_0)$ being linearly independent solutions of $H_0^* \psi(z_0) = z_0 \psi(z_0)$,

$$\lambda(z)_{ij}^{-1} = \lambda'(z)_{ij}^{-1} - (z - z') (\psi_j(\bar{z}), \psi_i(z')), \quad i, j \in 1, \dots, m.$$

Now we can finally formulate the main claim of this section.

Theorem 2.1.7. (*essential spectrum of quantum graphs with finitely many edges*)
Let Γ be a quantum graph with M internal and $N > 0$ external edges. Let H be a Hamiltonian defined in the first chapter with potential supported only on the internal edges. Then essential (and also absolutely continuous) spectrum of H is $[0, \infty)$.

Proof. For the proof one can use Weyl's theorem 2.1.5 and compare the resolvent of H with the resolvent of operator H_D which is obtained from H by replacing all coupling conditions by Dirichlet ones. Since both H and H_D are selfadjoint extensions of the same operator, it follows from the Krein's formula that the difference of their resolvents is a compact operator. Hence by theorem 2.1.5 the essential (and also absolutely continuous) spectrum of H is equal to the essential spectrum of M halflines with Dirichlet coupling condition at their ends. \square

A different situation can occur in the case with infinitely many internal edges. As for example Kronig-Penney model shows, there might be gaps in the continuous spectrum. Hence the previous result does not hold for section 3.4, as we consider there infinite tree graphs.

2.2 External complex scaling and resolvent poles

A very effective way how to study poles of the meromorphic continuation of the resolvent is the method of external complex scaling. The idea due to Augular and Combes [AC71, BC71] is to express resonances as eigenvalues of a scaled, nonselfadjoint operator. The scattering solution e^{ikx} , which does not belong to $L^2(\mathbb{R}_+)$, becomes under the scaling transformation square integrable.

The transformation of the wavefunction on the halflines is chosen to be

$$U_\theta g(x) = e^{\theta/2} g(e^\theta x). \quad (2.1)$$

If one chooses a real θ , then U_θ is a unitary operator which rescales the halflines. On the other hand, for nonreal θ the Hamiltonian on the graph H is transformed to a non-selfadjoint one.

Theorem 2.2.1. *Let H be a selfadjoint Hamiltonian on the graph acting as $-d^2/dx^2$ and as $-d^2/dx^2 + V_j(x)$ on the j -th internal edge. The transformed Hamiltonian acts as*

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

Proof. The result can be straightforwardly obtained applying transformation (2.1) to the elements on the semiinfinite leads.

$$\begin{aligned} U_\theta(-d^2/dx^2)U_{-\theta}g_j(x) &= U_\theta(-d^2/dx^2)e^{-\theta/2}g_j(e^{-\theta}x) = \\ &= U_\theta e^{-2\theta}e^{-\theta/2}g_j''(e^{-\theta}x) = e^{-2\theta}e^{-\theta/2}g_j''(e^{-\theta}x) = e^{-2\theta}g_j''(x). \end{aligned}$$

\square

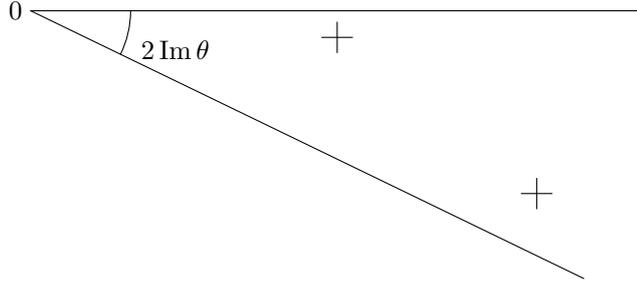


Figure 2.1: Spectrum of H_θ

Our aim is to transform outgoing scattering solutions into square integrable functions. Hence corresponding resonance energy becomes eigenvalue of H_θ . The spectral properties of operator H_θ are given in the following theorem.

Theorem 2.2.2. *The essential spectrum of H_θ is $e^{-2\theta}[0, \infty)$. The resonances of H can be obtained as eigenvalues of H_θ for $\text{Im } \theta$ large enough.*

Proof. Let $H_{D\theta}$ be defined as operator H_θ with coupling conditions changed to Dirichlet ones. Using the Krein's formula (theorem 2.1.6) and Weyl's theorem (theorem 2.1.5) we get that essential spectra of both operators are equal. Hence essential spectrum of H_θ is equal to essential spectrum M halflines rotated by the angle $e^{-2\theta}[0, \infty)$.

Let k be a resonance of H , i.e. there exists a non- L^2 solution of the Schrödinger equation on the graph with outgoing waves on the halflines. For simplicity, we take θ pure imaginary $\theta = i\vartheta$, $\vartheta \in (0, \pi)$ and large enough $-\vartheta < \text{Arg } k < 0$. Hence $g_{j\theta}(x) = g_j(0) e^{i\vartheta/2} \exp(ik e^{i\vartheta} x)$ is for $\text{Im}(k e^{i\vartheta}) > 0$ square integrable. One can straightforwardly check that function given on external leads by $g_{j\theta}(x)$ and on internal edges by $f(x)$ is eigenfunction of H_θ . Converse can be obtained similarly. \square

We give a very simple example of a quantum graph with nontrivial resonance condition to show how the above developed method works.

Example 2.2.3. *(a line with an appendix – resolvent resonances)*

The graph (see figure 2.2) consists of an abscissa of length l and a semiinfinite lead. The abscissa has Dirichlet condition at one end and is via δ -coupling of strength α connected with the halfline. 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 the Ansatz for solutions of the Schrödinger equation as

$$f(x) = ae^{-ikx} + be^{ikx}, \quad g(x) = ce^{-ikx} + de^{ikx}.$$



Figure 2.2: Example: a halfline with an appendix

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

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

The coupling conditions can be rewritten as

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

which leads to the resonance condition

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

2.3 Scattering matrix

A compact part of a quantum graphs with semiinfinite leads attached can be naturally seen as a scattering center. We define a scattering matrix similarly to e.g. [KS99] as an operator which maps the vector of incoming waves into the vector of outgoing waves. Since we do not assume any potential on the external edges, the solutions can be expressed as a combination of waves e^{ikx} and e^{-ikx} .

First, we elucidate why e^{-ikx} and e^{ikx} should be called incoming and outgoing solution, respectively. The motivation comes from the time dependent scattering problem. For simplicity, let us consider a time-dependent Schrödinger equation on a halfline $(-\partial_x^2 - i\partial_t)u_j(x, t) = 0$. Separating variables one can find its solution in the form $u_j(x, t) = e^{-itk^2} g_j(x)$, where $g_j(x)$ solves time-independent Schrödinger equation. Hence $u_j(x) = c_j e^{-ik(x+kt)} + d_j e^{ik(x-kt)}$. To make the argument of the first exponential constant for increasing t and positive real k , one needs to decrease x – the wave travels to the beginning of the halfline. Similarly, we can argue that the second term corresponds to the outgoing wave. A more exact definition is given below.

Definition 2.3.1. *Let us assume a quantum graph with M infinite leads ($0 < M < \infty$) parametrized by \mathbb{R}_+ . Let $\{c_j(k)\}_{j=1}^M$ be amplitudes of waves e^{-ikx} and $\{d_j(k)\}_{j=1}^M$ amplitudes of waves e^{ikx} . Then the scattering matrix is $M \times M$ matrix defined by its action $S(k)\{c_j(k)\} = \{d_j(k)\}$.*

Remark 2.3.1. We stress that our convention differs from the one usually used in the case $M = 2$. Natural approach in the case of a potential on the real line is to parametrize the halflines by \mathbb{R}_+ and \mathbb{R}_- (see e.g. [SZ91]). The incoming wave on \mathbb{R}_- is, of course, e^{ikx} which leads to switching the columns of the scattering matrix in comparison with our case.

The scattering matrix is unitary for real k 's, but for complex energies its entries can have poles. Writing down the equations for wave amplitudes which are sewed together at the vertices by coupling conditions and then separating out amplitudes of the solutions on the internal edges one obtains the set of equations

$$A(k)\{c_j(k)\} = B(k)\{d_j(k)\},$$

from which one simply gets the S-matrix as $S(k) = B(k)^{-1} \cdot A(k)$. The scattering poles can be obtained as poles of meromorphic continuation of the function $\det A(k)/\det B(k)$.

Despite the fact that “real physics occurs at real energies”, the resonances can be experimentally determined. If a pole of the S-matrix is close to the real axis, it can be determined from the peaks of the elements of the S-matrix for close real energies. In the time-dependent case it corresponds to the particle which resonates in the central part of the graph for time proportional to the reciprocal distance from the axis of reals.

We now give a theorem on the S-matrix which follows from results of section 3.1 and appendix A.

Theorem 2.3.2. (*explicit formula for the S-matrix of a general graph*)

Let Γ be a flower-like quantum graph without potential and with $2N$ internal and M external edges and the coupling given by unitary matrix U consisting of blocks U_1, \dots, U_4 (see also following section). Then S-matrix is a $M \times M$ matrix which can be written as

$$S(k) = F(k)^{-1} \cdot F(-k),$$

where $M \times M$ matrix $F(k)$ can be written as

$$F(k) = F_{21}(k)F_{11}(k)^{-1}F_{12}(k) - F_{22}(k)$$

with $F_{11}(k) = (U_1 - I)\tilde{C}_1(k) + ik(U_1 + I)\tilde{C}_2(k)$, $F_{12}(k) = U_{12}(1 + ik)$, $F_{21}(k) = U_{21}(\tilde{C}_1(k) + ik\tilde{C}_2(k))$ and $F_{22}(k) = (U_{22} - I) + ik(U_{22} + I)$. Matrices $\tilde{C}_1(k)$ and $\tilde{C}_2(k)$ are first $2N \times 2N$ blocks of matrices $C_1(k)$ and $C_2(k)$ defined in section 3.1 and appendix A.

Proof. The proof follows notation and some results of section 3.1 and appendix A. From the last unlabeled equation before equation 9 in appendix A we have

$$\begin{aligned} F_{11}(k)\vec{a} + F_{12}(k)\vec{d} &= F_{12}(-k)\vec{c}, \\ F_{21}(k)\vec{a} + F_{22}(k)\vec{d} &= F_{22}(-k)\vec{c}, \end{aligned}$$

where \vec{d} is the vector of amplitudes of the outgoing waves, \vec{c} is the vector of amplitudes of the incoming waves and \vec{a} corresponds to the internal parameter. The formula can be obtained straightforwardly if one takes corresponding Ansatzes on the internal and external edges and binds them with coupling conditions. After eliminating \vec{a} we get

$$(F_{21}(k)F_{11}(k)^{-1}F_{12}(-k) - F_{22}(-k))\vec{c} = (F_{21}(k)F_{11}(k)^{-1}F_{12}(k) - F_{22}(k))\vec{d}.$$

To complete the proof we have to check that $F_{21}(k)F_{11}(k)^{-1}$ is even in k . First, we notice that odd columns of $\tilde{C}_1(k)$ are odd in k and even columns even in k . The same holds true for the matrix $ik\tilde{C}_2(k)$. If one chooses arbitrary regular $2N \times 2N$ matrix $Q(k)$ with odd rows odd in k and even rows even in k then all entries of $F_{11}(k)Q(k)$ are even in k . Then we have

$$\begin{aligned} F_{21}(k)F_{11}(k)^{-1} &= F_{21}(k)(F_{11}(k)Q(k)Q(k)^{-1})^{-1} = \\ &= U_{21}(\tilde{C}_1(k) + ik\tilde{C}_2(k))Q(F_{11}(k)Q(k))^{-1}. \end{aligned}$$

Since both $(\tilde{C}_1(k) + ik\tilde{C}_2(k))Q$ and $F_{11}(k)Q(k)$ are even in k , also $F_{21}(k)F_{11}(k)^{-1}$ is even in k . The formula for the S-matrix follows from its definition. \square

Finally, in the example examined already in the previous section we show how scattering resonances can be obtained.

Example 2.3.3. *(a halfline with an appendix – scattering resonances)*

Let us assume the same example of a graph as in example 2.2.3. We again denote the components of the wavefunction by $f(x)$ and $g(x)$ respectively and impose Dirichlet condition on one end of the abscissa and Kirchhoff condition connecting the halfline and the abscissa.

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

Using the Ansatz $f(x) = ae^{-ikx} + be^{ikx}$ and $f(x) = ce^{-ikx} + de^{ikx}$ one obtains

$$\begin{aligned} a + b &= 0, \quad a(e^{-ikl} - e^{ikl}) = c + d, \\ ik(d - c) + ka(e^{-ikl} + e^{ikl}) &= \alpha(d + c). \end{aligned}$$

We finally obtain:

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

2.4 Effective coupling on a finite graph

In this section we introduce a simple construction which replaces the task of finding resonances of a quantum graph with attached halflines with solving Schrödinger equation on a compact part of the graph with energy dependent coupling conditions. This construction will be useful in the following chapters.

Let us assume a quantum graph with N internal and M external edges with coupling in the flower-like setting described by an unitary matrix U . We also assume that its columns and rows are arranged in the way that first $2N$ correspond to the internal edges and last M to the external ones. Let us write

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

where the $2N \times 2N$ block U_1 corresponds to the coupling between internal edges, $M \times M$ block U_4 couples external edges between each other and rectangular matrices U_2 and U_3 correspond to the coupling between internal and external edges. Then the condition 1.2 becomes

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

where I_n denotes $n \times n$ unit matrix, \vec{f} and \vec{g} denote the vectors of functional values from the internal and external edges, respectively, and \vec{f}' and \vec{g}' corresponding vectors of outward derivatives. After performing external complex scaling and replacing \vec{g} and \vec{g}' by $e^{-\theta/2}\vec{g}_\theta$ and $ike^{-\theta/2}\vec{g}'_\theta$, respectively, (see e.g. example 2.2.3) we can write

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

Now we can eliminate \vec{g}_θ and for $\det((1-k)U_4 - (k+1)I_M) \neq 0$ and write

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

which is formally the same equation as (1.2) only with U replaced by

$$\tilde{U}(k) = U_1 - I_{2N} - (1-k)U_2[(1-k)U_4 - (k+1)I_M]^{-1}U_3.$$

Theorem 2.4.1. (*effective coupling*)

Let H be a Schrödinger operator on a quantum graph Γ with $2N$ internal and M external edges and coupling given by $(2N + M) \times (2N + M)$ unitary matrix U consisting of blocks U_1 , U_2 , U_3 and U_4 (see above). Let $\{\lambda_i\}_{i=1}^M$ be eigenvalues of U_4 . Then all resolvent resonances of Γ on $\mathbb{C} \setminus \{\frac{\lambda_1-1}{\lambda_1+1}, \dots, \frac{\lambda_M-1}{\lambda_M+1}\}$ 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

$$\tilde{U}(k) = U_1 - (1-k)U_2[(1-k)U_4 - (k+1)I_M]^{-1}U_3. \quad (2.2)$$

Proof. The proof follows from the above construction. One only has to exclude the set given by zeros of determinant $\det((1-k)U_4 - (k+1)I_M)$. It is easy to check that the set $\{\frac{\lambda_1-1}{\lambda_1+1}, \dots, \frac{\lambda_M-1}{\lambda_M+1}\}$ does the job. \square

Typical situation which is not covered by the effective coupling is a resonance coming from a halfline separated from the rest of the graph with Robin condition on its end.

2.5 Equivalence of resolvent and scattering resonances

We formulate a theorem on relationship between resolvent and scattering resonances. It states equivalence of the two notions up to eigenvalues with corresponding eigenfunctions supported on the internal edges only.

Theorem 2.5.1. (*equivalence of resonances*)

Let Γ be a quantum graph with finite and infinite edges. Let the set of resolvent resonances be \mathcal{R}_R , the set of scattering resonances \mathcal{R}_S and the set of eigenvalues with eigenfunction supported on the compact part of Γ be \mathcal{R}_C . Then $\mathcal{R}_R = \mathcal{R}_S \cup \mathcal{R}_C$.

Proof. We use notation of the section 2.3 and denote by \vec{c} the vector of amplitudes of the incoming and by \vec{d} the vector of amplitudes of the outgoing waves on the external edges. Let us denote the two independent solutions on the j -th edge by u_j and v_j and coefficients of u_j and v_j by a_{j1} and a_{j2} , respectively. Hence the internal parameters of the solution are given by the vector $\vec{a} = \{a_{11}, a_{12}, \dots, a_{2N1}, a_{2N2}\}$. The coupling conditions at the vertices combined with the expression for functional values and derivatives at the vertices lead to the set of equations

$$(M_1(k) \quad M_2(k) \quad M_3(k)) (\vec{a}, \vec{c}, \vec{d})^T = 0,$$

where $M_1(k)$ is a $(2N + M) \times 2N$ matrix, and $M_2(k)$ and $M_3(k)$ are both $(2N + M) \times M$ matrices. k is an eigenvalue with compactly supported eigenfunction iff rank of $M_1(k)$ is smaller than $2N$. If it is not the case, one can perform such elementary row operations that the $M \times M$ submatrix in the left top corner of $M(k)'$ is regular. Suppose that after these row operation we obtain the matrix

$$M'(k) = \begin{pmatrix} M'_{11} & M'_{12} & M'_{13} \\ M'_{21} & M'_{22} & M'_{23} \end{pmatrix}.$$

Matrices M'_{ij} are in general, of course, energy-dependent, but for the sake of simplicity we do not explicitly mark their dependence on k . Separating \vec{d} and using the regularity of M'_{11} one gets

$$(M'_{22} - M'_{21}M'_{11}{}^{-1}M'_{12})\vec{c} + (M'_{23} - M'_{21}M'_{11}{}^{-1}M'_{13})\vec{d} = 0.$$

As we saw in the section 2.2, the resolvent resonances can be obtained as such k 's for which there exists solution with outgoing asymptotics. Hence we have $\det \begin{pmatrix} M'_{11} & M'_{13} \\ M'_{21} & M'_{23} \end{pmatrix} = 0$. For $M'_{11} \neq 0$ the previous condition is equal to vanishing of the determinant of the matrix before \vec{d} . From the theorem 2.3.2 follows $S(k) = F(k)^{-1} \cdot F(-k)$. Hence for $k \in \mathbb{C}_-$ for which $\det F(k) = 0$ there is no possibility of having $\det F(-k) = 0$ since that would mean a nonreal eigenvalue.

An explicit construction of matrix $M(k)$ can be found in appendix A. \square

2.6 Weyl's law of asymptotics

A lot of attention in the following chapter will be paid to the asymptotical behaviour of resonances. We now give an overview of the asymptotics of eigenvalues for Laplacians on a compact domain. The comparison to the asymptotical behaviour of resolvent resonances will be made in the following chapter.

The fundamentals of the theory were laid down by the seminal work of Weyl [Wey11] in which Sturm-Liouville operators on a bounded two-dimensional domain of area Ω and Dirichlet boundary condition were studied. If we define a counting function $N(\lambda)$ as the number of eigenvalues with absolute value smaller than λ , then

$$N(\lambda) = \frac{|\Omega|}{4\pi} \lambda.$$

Since then this law has been generalized to other dimensions and additional terms have been estimated. We give a result of Ivrii [Ivr80] for eigenvalues of a Laplace-Beltrami operator on a d -dimensional compact Riemannian C^∞ manifold

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

where ω_d stands for the volume of a d -dimensional ball with radius 1.

We will focus on the one-dimensional case, where the formula reads as follows. Let Γ be a compact quantum graph with the sum of lengths of all edges $V = \sum_i l_i$. Then the number of its eigenvalues in absolute value smaller than λ behaves asymptotically for $\lambda \rightarrow \infty$ as

$$N(\lambda) = \frac{V}{\pi} \lambda + o(1).$$

If one studies the same problem in the k -plane, one counts every eigenvalue twice since $k^2 = (-k)^2$. Hence there is an additional factor of two in the asymptotics formula.

A detailed introduction to the matter of Weyl's law and spectral properties of Laplacians can be found e.g. in [ANPS09]. Asymptotics of resonances is in detail studied in sections 3.2 and 3.3 and appendices B and C.

Chapter 3

Results

3.1 Resonances from perturbations of quantum graphs with rationally related edges

Let us assume a quantum graph without potential and with δ coupling conditions at the vertices which contains a loop of edges with lengths equal to some multiple of l_0 . Then clearly a function which is sine with zeros at the vertices of the loop and trivial outside the loop is an eigenfunction of H corresponding to eigenvalues $(n\pi)^2/l_0^2$, $n \in \mathbb{N}$ (see figure 3.1).

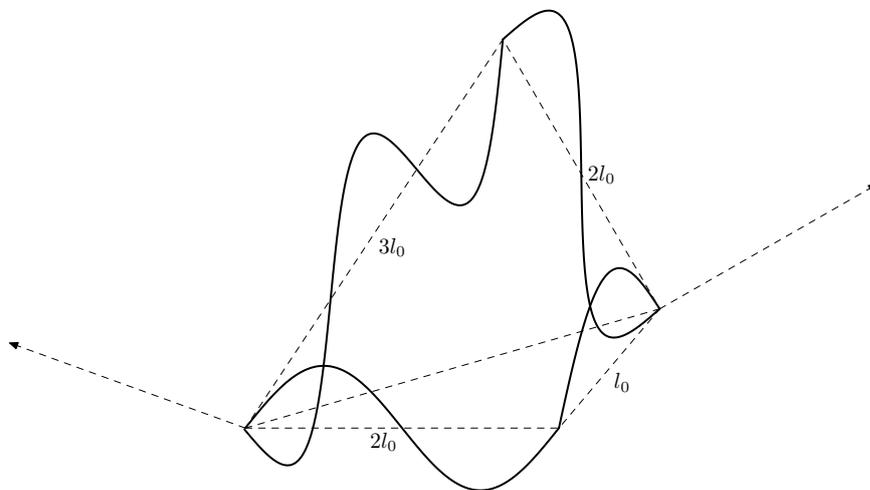


Figure 3.1: An example of an eigenfunction for a graph with rationally related edges

First, we give an explicit expression for the resonance condition for a graph without potential which has N internal and M external edges. It can be obtained using the procedure of external complex scaling and standard Ansatz on the edges.

$$\det [(U - I) C_1(k) + ik(U + I) C_2(k)] = 0 \quad (3.1)$$

where $C_1(k) = \text{diag}(C_1^{(1)}(k), C_1^{(2)}(k), \dots, C_1^{(N)}(k), I_{M \times M})$,
 $C_2(k) = \text{diag}(C_2^{(1)}(k), C_2^{(2)}(k), \dots, C_2^{(N)}(k), iI_{M \times M})$, respectively,

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

and $I_{M \times M}$ is a $M \times M$ unit matrix.

The following theorem gives sufficient condition on the coupling when eigenvalues with $kl_0 = 2\pi$ are present. It can be obtained from a relation similar to (3.1).

Theorem 3.1.1. *Let a graph Γ be a flower-like graph with N internal and M external edges with coupling given by unitary matrix U and condition (1.2). Let the lengths of the first n edges be integer multiples of a positive real number l_0 . If the rectangular $2N \times 2n$ matrix*

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

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

A similar theorem can also be stated for eigenvalues $\epsilon = (2m + 1)^2\pi^2/l_0^2$ with $m \in \mathbb{N}$, we refer the reader to appendix A.

The algebraic multiplicity of eigenvalues is given by the following theorem; again a similar one can be stated for odd eigenvalues.

Theorem 3.1.2. *In the setting of Theorem 3.1.1 suppose that the rank of M_{even} is smaller than $2n$. Let us vary the edge lengths, $l'_j = l_0(n_j + \varepsilon_j)$ with sufficiently small ε_j 's; then the multiplicity of the eigenvalues $\epsilon = k_0^2 = 4m^2\pi^2/l_0^2$ due to rationality of the first n edges is given by the difference between $2n$ and the rank of the matrix*

$$M_{\text{even}}^{\{\varepsilon_j\}} = \begin{pmatrix} u_{11} + \tilde{\varepsilon}_1^a & u_{12} - 1 + \tilde{\varepsilon}_1^b & u_{13} & u_{14} & \cdots & u_{1,2n-1} & u_{1,2n} \\ u_{21} - 1 + \tilde{\varepsilon}_1^b & u_{22} + \tilde{\varepsilon}_1^a & u_{23} & u_{24} & \cdots & u_{2,2n-1} & u_{2,2n} \\ u_{31} & u_{32} & u_{33} + \tilde{\varepsilon}_2^a & u_{34} - 1 + \tilde{\varepsilon}_2^b & \cdots & u_{3,2n-1} & u_{3,2n} \\ u_{41} & u_{42} & u_{43} - 1 + \tilde{\varepsilon}_2^b & u_{44} + \tilde{\varepsilon}_2^a & \cdots & u_{4,2n-1} & u_{4,2n} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ u_{2N-1,1} & u_{2N-1,2} & u_{2N-1,3} & u_{2N-1,4} & \cdots & u_{2N-1,2n-1} & u_{2N-1,2n} \\ u_{2N,1} & u_{2N,2} & u_{2N,3} & u_{2N,4} & \cdots & u_{2N,2n-1} & u_{2N,2n} \end{pmatrix},$$

where

$$\tilde{\varepsilon}_j^a(k) := \frac{(1 - k_0^2) \sin k_0 l_0 \varepsilon_j}{2ik_0 \cos k_0 l_0 \varepsilon_j - (1 + k_0^2) \sin k_0 l_0 \varepsilon_j}, \quad \tilde{\varepsilon}_j^b(k) := \frac{2ik_0(-1 + \cos k_0 l_0 \varepsilon_j) - (1 + k_0^2) \sin k_0 l_0 \varepsilon_j}{2ik_0 \cos k_0 l_0 \varepsilon_j - (1 + k_0^2) \sin k_0 l_0 \varepsilon_j}.$$

Finally, we present a result on local conservation of resolvent resonances.

Theorem 3.1.3. *Let Γ be a flower-like quantum graph with N finite edges of the lengths l_i , M infinite edges, and the coupling described by the matrix $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$, where U_4 corresponds to the coupling between the infinite edges. Let k_0 satisfy $\det[(1 - k_0)U_4 - (1 + k_0)I] \neq 0$ and let k_0 be a pole of the resolvent $(H - \lambda \text{id})^{-1}$ of a multiplicity d . Let Γ_ε be a geometrically perturbed quantum graph with the edges of lengths $l_i(1 + \varepsilon)$ and the same coupling as Γ . Then there exists an $\varepsilon_0 > 0$ such that 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 .*

In two particular examples we obtained trajectories of resolvent resonances. For more details we refer again to appendix A.

3.2 Non-Weyl asymptotics for quantum graphs with general coupling conditions

In appendix B attention is paid to the asymptotical behaviour of the number of resonances. For the purpose of this and the following section we denote by the term “resonances” all poles of the meromorphic continuation of the resolvent, i.e. both eigenvalues and “pure” resonances. The notion we are interested in is the number of resonances enclosed in a circle of diameter R in the k -plane. If one attaches several halflines to a compact graph and applies coupling conditions which separate the halflines from the compact part, then the set of resolvent resonances consists of eigenvalues with corresponding eigenfunctions supported on the compact part of the graph and a finite number of resonances coming from the halflines. It is natural to suppose that trajectories of resonances continuously depend on the coupling parameters. Hence we can use the results of section 2.6 and expect that following asymptotics will be satisfied.

$$N(R) = \frac{2V}{\pi}R \tag{3.2}$$

where V is the total size of the graph – the sum of lengths of the internal edges. We will call this asymptotics as *Weyl*. We again remind that the factor of two is due to “double counting” of resonances in the k -plane.

However, there are cases of graphs where this asymptotical behaviour is not fulfilled. One of them is sketched in figure 3.2. If we impose Kirchhoff (free) coupling conditions in all the vertices of graph in figure 3.2, the asymptotics of resonances satisfies linear dependence on R , but with different constant than in (3.2). We will refer to this type of behaviour as *non-Weyl*.

The reason is very simple. The coupling condition at the last vertex on the right assumes continuity of both the functional value and the derivative, hence one can replace the abscissa and the halfline by one halfline. Therefore the size of the graph can be effectively reduced.

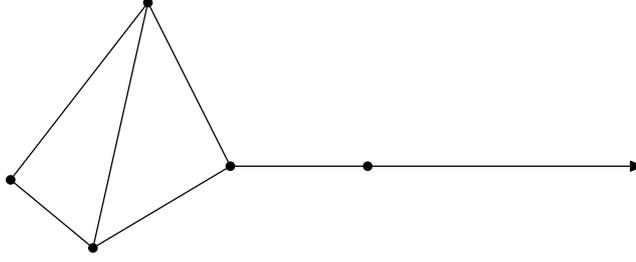


Figure 3.2: A trivial example of a non-Weyl graph

In the paper [DP11] Davies and Pushnitski extended this observation to all graphs with Kirchhoff coupling conditions stating a very simple geometric condition when the graph is non-Weyl. For its proof results of Langer [Lan31] on the number of zeros of exponential polynomials can be used.

Theorem 3.2.1. (*non-Weyl graphs for Kirchhoff conditions*)

Let Γ be a quantum graph with Kirchhoff coupling conditions and the sum of lengths of all internal edges V . Then the asymptotics of its resonances for $R \rightarrow \infty$ follows the rule

$$N(R) = \frac{2W}{\pi}R$$

with $0 \leq W \leq V$. The graph is non-Weyl ($W < V$) iff it has at least one balanced vertex. By a balanced vertex we denote a vertex connecting the same number of internal and external edges.

The main task of the paper in appendix B is to extend their result to all possible coupling conditions. It is not difficult to see that such a simple geometric condition as in Kirchhoff's case does not hold any longer. (For example, one can add several halflines with Dirichlet coupling conditions to a given vertex. This changes the ratio of internal and external edges, but does not add any resonances.) Instead, we use eigenvalues of the effective coupling matrix to distinguish Weyl and non-Weyl behaviour.

Theorem 3.2.2. (*non-Weyl graphs for general coupling conditions*)

Let Γ be a quantum graph, U unitary matrix describing the coupling on Γ and $\tilde{U}(k)$ effective coupling matrix defined by relation (2.2). Then Γ is non-Weyl iff $\tilde{U}(k)$ contains eigenvalues $\frac{1+k}{1-k}$ or $\frac{1-k}{1+k}$.

The proof of the theorem uses also properties of the exponential polynomials. The relationship between the eigenvalues of \tilde{U} and the example in figure 3.2 is simple. When one internal and one external edge is connected in the given vertex, the effective (in this case 1×1) coupling matrix $\tilde{U}(k)$ is equal to $\frac{1-k}{1+k}$ iff the coupling is Kirchhoff and $\tilde{U}(k) = \frac{1+k}{1-k}$ for its counterpart which we call "anti-Kirchhoff". However, these two possibilities of coupling are exceptional. We show in detail in appendix B that for permutation symmetric coupling the following theorem holds.

Theorem 3.2.3. (non-Weyl graphs for permutation symmetric coupling)

Let Γ be a graph with permutation symmetric coupling. It is non-Weyl iff there exist a vertex in which both following conditions are satisfied.

1. the vertex is balanced
2. the coupling is Kirchhoff ($U = \frac{1}{n}J - I$) or “anti-Kirchhoff” ($U = -\frac{1}{n}J + I$)

If a graph contains a balanced vertex connecting one halfline and one internal edge by Kirchhoff coupling, the non-Weyl behaviour of such a graph is obvious, since the internal edge can “be deleted” by the halfline. For a nontrivial non-Weyl graph, one can explicitly construct a unitary equivalent one in which this deletion is possible. The construction, which slightly generalizes the results of appendix B, is given in the theorem 3.2.4.

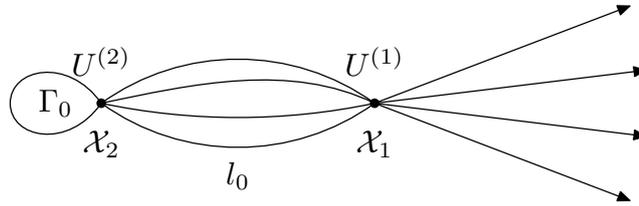


Figure 3.3: Construction of a unitarily equivalent graph

First we show that every quantum graph can be regarded as a graph in figure 3.3. Let us suppose that we have a flower-like graph with central vertex \mathcal{X}_1 and the smallest edge of length $2l_0$ and coupling matrix $U^{(1)}$. We introduce additional vertices with Kirchhoff coupling conditions on each edge in distance l_0 from \mathcal{X}_1 , then we connect all of them together to the vertex \mathcal{X}_2 as in the flower like model and we denote the coupling matrix in \mathcal{X}_2 by $U^{(2)}$.

Theorem 3.2.4. (construction of a unitarily equivalent graph)

Let Γ be previously described graph in figure 3.3 consisting of M internal edges, $2N$ links between \mathcal{X}_1 and \mathcal{X}_2 and the rest of the graph Γ_0 having $P < N$ edges. We suppose that for Hamiltonian H_1 the coupling is described by matrices $U^{(1)}$ and $U^{(2)}$. For any $M \times M$ unitary matrix V_2 and $2N \times 2N$ unitary matrix V_1 we define $V^{(1)} = \begin{pmatrix} V_2 & 0 \\ 0 & V_1 \end{pmatrix}$, $V^{(2)} = \begin{pmatrix} I_P & 0 \\ 0 & V_2 \end{pmatrix}$ and subsequently Hamiltonian H_2 which differs from H_1 by replacing the coupling matrices $U^{(1)}$ and $U^{(2)}$ by $V^{(1)-1}U^{(1)}V^{(1)}$ and $V^{(2)-1}U^{(2)}V^{(2)}$, respectively. Then H_2 is unitarily equivalent to H_1 .

Proof. Let u be an element of the domain of H_1 and u_1, \dots, u_{2N} its restrictions to the internal edges between \mathcal{X}_1 and \mathcal{X}_2 , f_1, \dots, f_M its restrictions to the infinite edges and u_0 its restriction to the rest of the graph Γ_0 . We define a map V from

the domain of H_1 to the domain of H_2 as follows.

$$\begin{aligned} (u_1, \dots, u_{2N})^T &\mapsto (v_1, \dots, v_{2N})^T = V_1^{-1}(u_1, \dots, u_{2N})^T, \\ (f_1, \dots, f_{2N})^T &\mapsto (g_1, \dots, g_{2N})^T = V_2^{-1}(f_1, \dots, f_{2N})^T, \\ u_0 &\mapsto v_0 = u_0. \end{aligned}$$

It is straightforward to check that V maps to the domain of H_1 into the domain of H_2 and that the coupling conditions are transformed into the above form. \square

In appendix B also the problem of determining the effective size of a non-Weyl graph is considered. The examined example is a regular polygon with two halflines attached at each vertex and Kirchhoff's coupling conditions. According to theorem 3.2.1 this graph is non-Weyl, since every vertex is balanced. We have elegant methods how to find a non-Weyl graph, but the task of determining its actual effective size is more complicated. The result for n internal edges of length l

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

shows that additional symmetry of a graph with $n \equiv 0 \pmod{4}$ allows us to “delete” more internal edges. This shows that in contrast to the type of asymptotics of the graph, which can be determined locally from characteristics of the vertex, the effective size is a global issue.

3.3 Non-Weyl resonance asymptotics for quantum graphs in a magnetic field

Appendix C addresses the question whether the asymptotics of resonances can be changed by putting the quantum graph into a magnetic field. The answer is both yes and no – it depends on precise statement of the question. The first main result is that a quantum graph with non-Weyl asymptotics cannot be using magnetic field turned into a Weyl graph and vice versa. On the other hand, if a graph is already non-Weyl, its “effective size” can be in some cases influenced by the presence of certain magnetic field.

The magnetic Hamiltonian we are dealing with acts as $-(d/dx + iA_j(x))^2$ at the internal edges and as negative second derivative at the external ones on functions from $W^{2,2}(\Gamma)$ satisfying slightly changed coupling condition (1.2)

$$(U - I)\Psi + i(U + I)(\Psi' + i\mathcal{A}\Psi) = 0$$

with $\text{diag}(A_1(0), -A_1(l_1), \dots, A_N(0), -A_N(l_N), 0, \dots, 0)$ being diagonal matrix with entries equal to limiting values of magnetic potential to the vertex.

Using a gauge transformation one can transform out the magnetic field. The price one pays for it is that coupling conditions must be changed accordingly. We obtain

$$(U_A - I)\Psi + i(U_A + I)\Psi' = 0, \quad U_A := \mathcal{F}U\mathcal{F}^{-1} \quad (3.3)$$

with $\mathcal{F} = \text{diag}(1, \exp(i\Phi_1), \dots, 1, \exp(i\Phi_N), 1, \dots, 1)$ containing magnetic fluxes $\Phi_j = \int_0^{l_j} A_j(x) dx$.

As stated in theorem 3.2.2 the fact whether the asymptotics is Weyl or non-Weyl is given by presence of particular eigenvalues of $\tilde{U}(k)$. Let us assume a unitary transformation $V^{-1}UV$ with V block diagonal in the way that it does not mix the coupling between internal and external edges. It can easily be seen from the form of equation (2.2) that $\tilde{U}(k)$ is also changed by unitary transformation and hence its eigenvalues are preserved. Since transformation (3.3) belongs to the above class, we arrive at the following claim.

Theorem 3.3.1. *Let Γ be a quantum graph without magnetic field and Γ_A the same graph placed into a magnetic field. Then Γ_A is non-Weyl iff Γ is.*

On the other hand, one can change the “effective size” of a non-Weyl graph by tuning the magnetic field. This effect is in the appendix C studied in detail for graphs with one loop. After explicitly expressing the resonance condition one can prove the following statement which imposes conditions on the nondiagonal terms of the effective coupling matrix.

Theorem 3.3.2. *The effective size of a graph with a single internal edge is zero iff it is non-Weyl and its effective coupling matrix $\tilde{U}(k)$ satisfies $\tilde{u}_{12} + \tilde{u}_{21} = 0$.*

The proof can be done by explicit computation of the resonance condition and getting rid of the term not depending on l . The term with e^{ikl} is already zero since we suppose non-Weyl asymptotics of the graph. The magnetic field can change the phase of the non-diagonal terms of the effective coupling matrix. Clearly, if $|u_{12}(k)| = |u_{21}(k)|$ one can choose such a magnetic flux through the loop that the condition of the above theorem is fulfilled. Hence every non-Weyl graph with $|u_{12}(k)| = |u_{21}(k)|$ has for a certain value of magnetic field zero effective size (i.e. finitely many resonances).

3.4 On the absence of absolutely continuous spectra for Schrödinger operators on radial tree graphs

The article in appendix D is different from the others since it deals with spectrum of a tree graph. It includes two main claims. First one establishes equivalence between Hamiltonian on tree graphs and an orthogonal sum of Hamiltonians on halflines. This is done for a large class of coupling conditions and it largely generalizes the result of Sobolev and Solomyak [SS02]. The second part is devoted to the study of the spectrum in the case when the graph is sparse. It uses previous construction of the unitary equivalence and generalizes the result by Breuer and Frank [BF09], who studied graphs with Kirchhoff coupling conditions. We give conditions under which the graph does not have absolutely continuous spectrum.

We also show that this claim is not trivial, since there exist such coupling conditions on the tree graph which can be mapped to the free halfline. Hence there exist examples of sparse tree graphs which do have (sometimes purely) absolutely continuous spectrum. Nevertheless, this class is exceptional.

We are interested in radial tree graphs. We assume a rooted tree graph; we say that a vertex belongs to the k -th generation if there are $k - 1$ vertices on the shortest path to the root. A tree graph is called *radial* if the branching number b_k (number of edges emanating from the vertex) is the same in the same generation and all edges of the same generation have equal length (see figure 3.4). The branching function is defined by $g_0(t) = b_0 b_1 \dots b_k$ if $t \in (t_k, t_{k+1})$ where t is the distance from the root and t_k determine the location of vertices (distance of the vertices in k -th generation from the root).

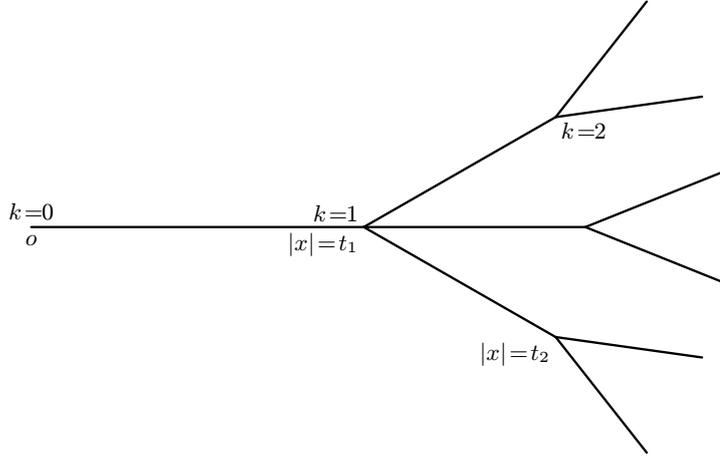


Figure 3.4: A radial tree graph

We introduce $[(b_k - 1)^2 + 4]$ -parameter class of coupling conditions. In general, coupling in the vertex of a k -th generation can be described by $(b_k + 1)^2$ parameters, we study its subclass which allows us to separate the symmetric part of the wavefunction from the antisymmetric part.

$$\sum_{j=1}^{b_k} f'_{vj+} - f'_{v-} = \frac{\alpha_{tk}}{2} \left(\frac{1}{b_k} \sum_{j=1}^{b_k} f_{vj+} + f_{v-} \right) + \frac{\gamma_{tk}}{2} \left(\sum_{j=1}^{b_k} f'_{vj+} + f'_{v-} \right),$$

$$\frac{1}{b_k} \sum_{j=1}^{b_k} f_{vj+} - f_{v-} = -\frac{\bar{\gamma}_{tk}}{2} \left(\frac{1}{b_k} \sum_{j=1}^{b_k} f_{vj+} + f_{v-} \right) + \frac{\beta_{tk}}{2} \left(\sum_{j=1}^{b_k} f'_{vj+} + f'_{v-} \right).$$

$$(U_k - I)V_k\Psi_v + i(U_k + I)V_k\Psi'_v = 0,$$

with

$$\Psi_v := (f_{v1+}, f_{v2+}, \dots, f_{vb_k+})^T,$$

$$\Psi'_v := (f'_{v1+}, f'_{v2+}, \dots, f'_{vb_k+})^T.$$

Here v denotes the vertex of the k -th generation, the signs $-$ and $+$ refer to the incoming edge and the edges emanating from the vertex, respectively. The subscript $j = 1, \dots, b_k$ distinguishes the emanating edges. The rectangular $b_k \times (b_k - 1)$ matrix V_k has orthonormal rows which are also orthonormal to the vector with all entries equal to 1. Symbol U_k denotes, as in previous sections, a unitary $(b_k - 1) \times (b_k - 1)$ matrix.

In the root we can choose arbitrary Robin coupling condition.

The unitary equivalence is established by the following theorem.

Theorem 3.4.1. *The Hamiltonian \mathbf{H} acting as minus second derivative on a radial tree graph Γ with the above coupling conditions is unitarily equivalent to*

$$\mathbf{H} \cong H_{L_0} \oplus \bigoplus_{n=1}^{\infty} \bigoplus_{s=1}^{b_n-1} (\oplus b_0 \dots b_{n-1}) H_{L_{n_s}}.$$

where $(\oplus m)H_{L_{n_s}}$ is the orthogonal sum of m identical copies of the operator on the halfline $H_{L_{n_s}}$. The Hamiltonian $H_{L_{n_s}}$ acts as minus second derivative on the halfline starting at t_n with the domain consisting of functions in $W^{2,2}((t_n, \infty))$ satisfying following coupling conditions at $t_k, k > n$.

$$\begin{aligned} y'_{k+} - y'_{k-} &= \frac{\alpha_{hk}}{2}(y_{k+} + y_{k-}) + \frac{\gamma_{hk}}{2}(y'_{k+} + y'_{k-}), \\ y_{k+} - y_{k-} &= -\frac{\tilde{\gamma}_{hk}}{2}(y_{k+} + y_{k-}) + \frac{\beta_{hk}}{2}(y'_{k+} + y'_{k-}), \\ y'_{n+} + y_{n+} \tan \frac{\theta_{n_s}}{2} &= 0, \end{aligned}$$

where

$$\alpha_{hk} := \frac{16\alpha_{tk}}{4(b_k^{1/2} + 1)^2 + \det \mathcal{A}_{tk}(b_k^{1/2} - 1)^2 + 4(1 - b_k) \operatorname{Re} \gamma_{tk}}, \quad (3.4)$$

$$\beta_{hk} := \frac{16 b_k \beta_{tk}}{4(b_k^{1/2} + 1)^2 + \det \mathcal{A}_{tk}(b_k^{1/2} - 1)^2 + 4(1 - b_k) \operatorname{Re} \gamma_{tk}}, \quad (3.5)$$

$$\gamma_{hk} := 2 \cdot \frac{(1 - b_k)(4 + \det \mathcal{A}_{tk}) + 8ib_k^{1/2} \operatorname{Im} \gamma_{tk} + 4(b_k + 1) \operatorname{Re} \gamma_{tk}}{4(b_k^{1/2} + 1)^2 + \det \mathcal{A}_{tk}(b_k^{1/2} - 1)^2 + 4(1 - b_k) \operatorname{Re} \gamma_{tk}},$$

$$\mathcal{A} = \begin{pmatrix} \alpha & \gamma \\ -\tilde{\gamma} & \beta \end{pmatrix}.$$

The proof uses the fact that the coupling conditions at the tree separate the symmetric and antisymmetric part of the wavefunction. One finds unitary equivalence of the symmetric subspace of the domain of \mathbf{H} with operator H_{L_0} taking into account the branching function. For the subspace of antisymmetric functions one proceeds similarly – one takes functions symmetric with respect to the vertices of the second generation and proceeds recursively.

The proof of the absence of the absolutely continuous spectrum uses the above decomposition. One needs to prove the absence of the absolutely continuous

spectrum for each halfline of the decomposition. The final result for tree graphs is obtained in the following theorem. Since the theorem is a bit technical, we first for brevity write down several conditions needed there.

$$\det \mathcal{A}_{t_n}(\sqrt{b_k} - 1) + 4(1 - b_n) \operatorname{Re} \gamma_{t_n} + 4(1 + \sqrt{b_n}) \neq 0 \quad (3.6)$$

$$\begin{aligned} \frac{1}{K} < & \left| 4 - 2\sqrt{b_n}(\det \mathcal{A}_{t_n} - 4) + \det \mathcal{A}_{t_n} \right. \\ & \left. + b_n(4 + \det \mathcal{A}_{t_n} - 4\operatorname{Re} \gamma_{t_n}) + 4\operatorname{Re} \gamma_{t_n} \right| < K \end{aligned} \quad (3.7)$$

$$\begin{aligned} \frac{1}{K} < & 4b_n \det \mathcal{A}_{t_n} + (1 - b_n)[(4 + \det \mathcal{A}_{t_n} + 4\operatorname{Re} \gamma_{t_n})^2 \\ & - b_n(4 + \det \mathcal{A}_{t_n} - 4\operatorname{Re} \gamma_{t_n})^2] < K \end{aligned} \quad (3.8)$$

$$\frac{b_n^{1/2}}{|\beta_{t_n}|} \sqrt{(-4 + \det \mathcal{A}_{t_n})^2 + (4 \operatorname{Im} \gamma_{t_n})^2} > 1/K \quad (3.9)$$

Theorem 3.4.2. *(absence of the absolutely continuous spectrum for graphs)*

Let \mathbf{H} be the Hamiltonian acting as $-d^2/dx^2$ on a radial tree graph with branching numbers b_n and the domain consisting of all functions $f \in \bigoplus_{e \in \mathcal{E}} H^2(e)$ satisfying the above coupling conditions at t_n , $n \in \mathbb{N}$, among which the number of separating ones is at most finite. Suppose that there are $K \in (0, \infty)$ and $N \in \mathbb{N}$ such that for all $n > N$ the following conditions hold:

- (i) $\limsup_{n \rightarrow \infty} (t_{n+1} - t_n) = \infty$,
- (ii) $\inf_{m,n} (t_m - t_n) > 0$,
- (iii) either $\operatorname{Im} \gamma_{t_n} \neq 0$, or both $\det \mathcal{A}_{t_n} \neq 4$ and condition (3.6) are valid,
- (iv) conditions (3.7) and (3.8) hold,
- (v) finally, one of the following conditions holds:
 - (a) $b_n |\beta_{t_n}| > \frac{1}{K}$ and (3.9) is valid for all $n > N$,
 - (b) $\beta_{t_n} = 0$, and either the right-hand side of (3.4) is larger than $1/K$ for all $n > N$ or smaller than $-1/K$ for all $n > N$, or the rhs of (3.5) is larger than $1/K$ for all $n > N$ or smaller than $-1/K$ for all $n > N$.

Then the absolutely continuous spectrum of \mathbf{H} is empty.

On the other hand, there exist examples of graphs with absolutely continuous spectrum. If one chooses the coupling on the tree with $\alpha_{t_n} = \beta_{t_n} = 0$, while $\gamma_{t_n} = 2 \frac{b_n^{1/2} - 1}{b_n^{1/2} + 1}$, then in the decomposition a free halfline appears. Hence the absolutely continuous part of the spectrum is nontrivial.

Conclusion

In the first two chapters we defined basic notions, introduced concepts used in the results and gave main theorems concerning quantum graphs. The third chapter summarized the main results of the theses, which are given in the appendices.

We have studied resonances coming from perturbation of graphs with rationally related edges, we gave conditions on the coupling for which there are certain eigenvalues embedded into the continuous spectrum. We proved that the number of resonances is locally conserved and in two examples we showed trajectories of such resonances.

We studied asymptotical behaviour of number of resonances for general quantum graphs. We gave a condition how to distinguish Weyl and non-Weyl behaviour and we explained non-Weyl behaviour by a construction of an equivalent graph. We showed that the non-Weyl behaviour is exceptional – the only options for a permutation symmetric coupling are the Kirchhoff and “anti-Kirchhoff” couplings. We also studied asymptotics for weighted graphs. We gave an expression for the effective size of the graph for a polygon showing that it depends on the structure of the whole graph.

In the case of magnetic quantum graphs we obtained two main results. Magnetic field cannot switch a non-Weyl graph into a Weyl one and vice versa. Despite of it, it is possible to effect by magnetic field the constant by the leading term of non-Weyl asymptotics. We showed that for one-loop non-Weyl graphs there always exists such a magnetic field for which the graph has finite number of resonances.

We established a unitary equivalence between Hamiltonians on radial tree graphs and orthogonal sum of Hamiltonians on halflines for a large class of coupling conditions. We showed that under some conditions sparse tree graphs do not have absolutely continuous spectrum. On the other hand, there still exist examples of non-trivial sparse graphs with purely absolutely continuous spectrum.

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List of Notation

α, β, γ	coupling parameters
Γ	quantum graph
H	the Hamiltonian
\mathcal{H}	Hilbert space
\mathcal{E}_i	the set of internal edges of a graph
\mathcal{E}_e	the set of external edges of a graph
I	unit matrix
J	matrix with all entries equal to one
Ker	kernel of an operator
$L^2(\Gamma)$	the space of square integrable functions
Ψ	the vector of functional values at the vertex of a graph
Ψ'	the vector of outgoing derivatives at the vertex of a graph
$R(\lambda)$	the resolvent
Ran	range of an operator
$S(k)$	the scattering matrix
U	the coupling matrix
$\tilde{U}(k)$	the effective coupling matrix for a compact graph
\mathcal{V}	the set of vertices
$V(x)$	the potential (on the internal edges of a graph)
V	the sum of the lengths of the internal edges of the graph
$W^{2,2}(\Gamma)$	the Sobolev space
\mathcal{X}_j	particular vertex of a graph

Attachments

Appendix A

Resonances from perturbations of quantum graphs with rationally related edges

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Appendix B

Non-Weyl asymptotics for quantum graphs with general coupling conditions

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Appendix C

Non-Weyl resonance asymptotics for quantum graphs in a magnetic field

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Appendix D

On the absence of absolutely continuous spectra for Schrödinger operators on radial tree graphs

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