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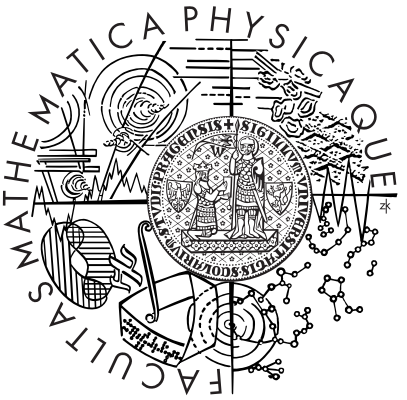

Jiří Lipovský

Spektrální a rezonanční vlastnosti kvantových grafů

Ústav teoretické fyziky

Vedoucí diplomové práce: Prof. RNDr. Pavel Exner, DrSc.,
Ústav jaderné fyziky, Akademie věd ČR
Studijní program: Fyzika, Teoretická fyzika

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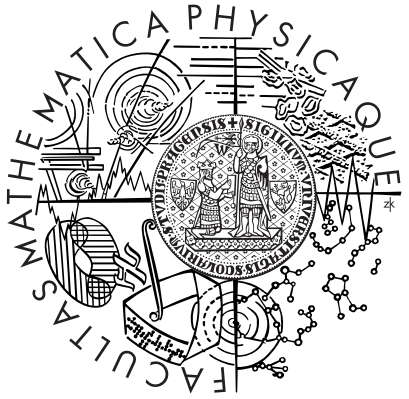

Jiří Lipovský

Spectral and resonance properties of quantum graphs

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Field of study: Physics, Theoretical physics

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Děkuji Prof. RNDr. Pavlu Exnerovi, DrSc. za odborné vedení, cenné rady a připomínky, které jsem uplatnil při psaní diplomové práce.

Prohlašuji, že jsem svou diplomovou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce a jejím zveřejňováním.

V Praze dne 18. 4. 2008 Jiří Lipovský

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Abstrakt: V této práci studujeme spektrální vlastnosti diferenciálního operátoru druhého řádu na kvantovém grafu. Věnujeme se několika problémům. Pro kvantový graf s racionálním poměrem délek jeho hran zkoumáme trajektorie rezonancí v případě, že poměr délek jeho hran je narušen. Dále studujeme strukturu spektrální variety a Berryho fázi pro hvězdicovitý graf. V poslední části dokážeme unitární ekvivalenci mezi hamiltoniánem na stromovém grafu a hamiltoniánem na polopřímce.

Klíčová slova: kvantové grafy, mezoskopické systémy, Berryho fáze.

Title: Spectral and resonance properties of quantum graphs
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Abstract: In the present work we study the spectral properties of a second-order differential operator on the quantum graph. We investigate several problems. For an quantum graph with the rational rate of the lenghts of its edges, we investigate the trajectories of the resonances when the lengths of the edges are perturbated. Furthermore, we study the topology of the spectral manifold and the Berry's phase for star graphs. In the last part, we prove the unitary equivalence between the Hamiltonian on the tree graph and the Hamiltonian on the halfline.

Keywords: quantum graphs, mesoscopic systems, Berry's phase.

Chapter 1

Introduction

Quantum graphs are a widely used model, mainly in the solid state physics. From the mathematical point of view, a quantum graph is a one-dimensional network structure, equipped with a selfadjoint second-order differential operator (negative Laplacian with a potential) with certain coupling conditions at the vertices; its analysis reduces to solving a system of ordinary differential equations.

A motivation comes from a more complicated model, the so-called *quantum wires* (see, e.g., [KuZ01]). Using the model of a quantum graph, one reduces the problem to one-dimensional one, neglecting the width of the wire. The aim is to study the motion of a quantum particle on this configuration space, under the influence of the electric or magnetic field. One can predict the conductance of the structure or other quantum effects. Another approach to quantum wire networks are the so-called *leaky graphs* (see, e.g., [E07]), where a negative multiple of the δ-distribution on the graph is added to the Laplacian and the partial corresponding differential equations are solved.

The first application of quantum graphs can be traced back to the 1950's. Ruedenberg and Scherr [RS53] used this model for describing the σ-electrons in aromatic organic molecules, the atoms were considered as the vertices of the graph.

In the last two decades, quantum graphs were studied more intensively, motivated by the progress in fabricating of the nanostructures consisting of quantum wires. The model is used in mesoscopic physics, nanotechnology or microelectronics. The *photonic crystals* (e.g., [KK02]) are a certain analogy of the electron motion in the semiconductor structures. They are periodic optical nanodevices, in which the motion of the photon is affected by the

change of the dielectric constant.

One of the virtues of quantum graphs is that they provide us with a simple framework to study the *quantum chaos*. The pioneering paper by Kottos and Smilansky [KoS97] shows that the spectral statistics of the quantum graphs is reproduced by the random matrix theory. Berkolaiko, Bogomolny and Keating have recently proved in the paper [BBK00] that the star graph has the same spectral statistics as Šeba billiards, an example of two-dimensional chaotical system. A review on statistics on quantum graphs can be found in [GS06].

Kostrykin and Schrader studied in [KS00] the inverse scattering problem on quantum graphs and provided a way to possible designing of elementary gates in quantum computing. A summary on quantum graphs can be found, e.g., in [KS99], [Ku04] or [GS06].

In the present work we try to contribute with the study of several spectral problems concerning quantum graphs. First, we introduce the model and some important common properties of quantum graphs. The next chapter investigates the resonances developing from eigenvalues embedded into the continuous spectrum of the graph with rational rate of the lengths of some edges due to the perturbation of lengths of these edges. After studying trajectories of the poles of the resolvent in two simple examples we formulate a theorem determining the number of the resonances for the general case. The next part of this work is devoted to the so-called star graphs (all their edges are connected at one endpoint). We study the structure of the spectral manifold and find the Berry's phase for the change of one of the parameters. The last part of the work is devoted to demonstrating the unitary equivalence between the Hamiltonian on some types of tree graphs and the Hamiltonian on the halfline which generalizes the Somomyak-Sobolev duality. We use it to derive spectral properties of regular tree graphs with a general coupling in the vertices.

Chapter 2

Preliminaries about quantum graphs

2.1 Description of the model

The configuration space of our model is a graph Γ, described by the set of vertices $\mathcal{V} = \{\mathcal{X}_j, j \in I\}$ and the set of edges $\mathcal{L} = \{\mathcal{L}_{jn} : (\mathcal{X}_j, \mathcal{X}_n) \in I_{\mathcal{L}} \subset I \times I\}$ attached to them, where I is a finite or countably infinite index set. Each edge can be identified by the pair of vertices (in any order, since the graph is not directed) and the length l_{jn} of each edge in $\mathcal{L}$ is positive. We suppose that to some vertices in $\mathcal{V}$ one or more semiinfinite external links are attached. We denote the whole graph by Γ and its subset with finite edges only by Γ_e.

The set of the vertices which are connected to the vertex $\mathcal{X}_j$ by an edge (its *neighbours*) is denoted by $\mathcal{N}(\mathcal{X}_j) = \{\mathcal{X}_n : n \in \nu(j) \subset I \backslash \{j\}\}$. We denote by $\mathcal{B}$ the set of vertices which have a single neighbour (*graph boundary*), its complement is called *graph interior* and is denoted by $\mathcal{I} = \mathcal{V} \backslash \mathcal{B}$. We denote by $\mathcal{C}$ the set of vertices to which one or more semiinfinite links are attached. Similarly, the corresponding index subsets are denoted by $I_{\mathcal{B}}$, $I_{\mathcal{I}}$, and $I_{\mathcal{C}}$.

Furthermore, the metric on the graph can be identified with a part of a Euclidean space. Using the metric structure, we introduce the Hilbert space of the problem

$$\mathcal{H} = \bigoplus_{(j,n) \in I_{\mathcal{L}}} L^2([0, l_{jn}]) \oplus \bigoplus_{j \in I_{\mathcal{C}}} L^2([0, \infty)).$$

The elements of $\mathcal{H}$ can be witten by $\psi = \{\psi_{jn} : (j,n) \in I_{\mathcal{L}},\ \psi_{j\infty} : j \in I_{\mathcal{C}}\}$.

Our aim is to describe quantum mechanics on such a graph. For simplicity, we choose the system of units where $\hbar^2 = 1$ and $2m = 1$. Furthermore, we define on the graph Γ the differential operator $H = -\mathrm{d}^2/\mathrm{d}x^2 + V(x)$ with essentially bounded potential

$$V = \{V_{jn}, V_{j\infty}\}, V_{jn} \in L^\infty([0, l_{jn}]), V_{j\infty} = 0\,.$$

The domain of definition of this Hamiltonian are functions ψ in the appropriate Sobolev space on the graph, i. e. $\psi_{jn} \in W^{2,2}([0, l_{jn}]), \psi_{j\infty} \in W^{2,2}([0, \infty))$, which satisfy suitable coupling condition at the vertices, to be described below.

2.2 Vertex coupling

Identifying the point $\mathcal{X}_j$ with $x = 0$ we denote the limits of functions and their derivatives on $\mathcal{L}_{jn}$ by

$$\psi_{jn} = \lim_{x \to 0+} \psi_{jn}(x)\,, \quad \psi'_{jn} = \lim_{x \to 0+} \psi'_{jn}(x)\,.$$

For each vertex $\mathcal{X}_j$ we denote by

$$\Psi_j = (\psi_1(\mathcal{X}_j), \psi_2(\mathcal{X}_j), \ldots, \psi_{d_j}(\mathcal{X}_j))^T, \quad d_j = \mathrm{card}\,\mathcal{N}(\mathcal{X}_j)$$

the column vector of function values at the point $\mathcal{X}_j$ and, similarly,

$$\Psi'_j = (\psi'_1(\mathcal{X}_j), \psi'_2(\mathcal{X}_j), \ldots, \psi'_{d_j}(\mathcal{X}_j))^T, \quad d_j = \mathrm{card}\,\mathcal{N}(\mathcal{X}_j)\,.$$

the vector of one-sided derivatives at $\mathcal{X}_j$.

We must ensure that the Hamiltonian is self-adjoint. The general coupling in a vertex $\mathcal{X}_j$ of a quantum graph can be described by two square $d_j \times d_j$ matrices

$$A_j \Psi_j + B_j \Psi'_j = 0\,, \tag{2.1}$$

such that the $d_j \times 2\,d_j$ matrix (A_j, B_j) has maximal rank and $A_j B_j^\dagger$ is self-adjoint at each vertex, where $\dagger$ means adjoint. This condition is equivalent to the self-adjointness of the Hamiltonian, this result was first obtained by Kostrykin and Schrader in [KS99].

Furthermore, the condition (2.1) can rewritten in the form (showed independently by Kostrykin and Schrader [KS00] and Harmer [Ha00]; in general context such condition were known earlier [GG91])

$$(U_j - I)\Psi_j + iL_0(U_j + I)\Psi'_j = 0\,, \tag{2.2}$$

where U_j is an arbitrary unitary $d_j \times d_j$ matrix, I is the unit $d_j \times d_j$ matrix and L_0 is a non-zero constant of length dimension. It only seems that L_0 adds an extra parameter (recall that a general self-adjoint extension is in this situation characterized by d_j^2 real parameters) because the conditions corresponding to different L_0, L_0' are mutually related by

$$U' = [(L_0 - L_0')U + (L_0 + L_0')]^{-1}[(L_0 + L_0')U + (L_0 - L_0')I]\,.$$

Hence without loss of generality we can take $L_0 = 1$. Therefore, the coupling at every vertex can be described by d_j^2 parameters. Notice that the coupling (2.1) has the same number of the degrees of freedom, because it is non-unique: the matrices A_j and B_j can be replaced by C_jA_j and C_jB_j, where C_j is an ordinary regular $d_j \times d_j$ matrix.

The relation between the matrices A_j, B_j and the unitary matrix U_j can be obtained from the equations

$$C_jA_j = U_j - I\,, \quad C_jB_j = i(U_j + I)\,.$$

Using linear combination of the previous equations one arrives at

$$2U_j = C_j(A_j - iB_j)\,, \quad 2I = -C_j(A_j + iB_j)$$

and hence one obtains the relation

$$-(A_j + iB_j)U_j = A_j - iB_j \tag{2.3}$$

or an equivalent one

$$(B_j - iA_j)U_j = B_j + iA_j\,. \tag{2.4}$$

In particular, we mention several interesting cases of coupling

1. δ-coupling:

$$\begin{aligned} \psi_j := \psi_{jn}(j) &= \psi_{jm}(j) \quad \text{for all } n, m \in \nu(j)\,, \\ \sum_{n\in\nu(j)} \psi'_{jn}(j) &= \alpha_j\psi_j \end{aligned}$$

with $\alpha_j \in \mathbb{R}$. Let J be a $d_j \times d_j$ matrix with all entries equal to one. Then the matrices A_j and B_j can be chosen as $A_j = -\alpha I$, $B_j = J$. Since $J^2 = d_jJ$, the matrix U_j can be also chosen as a linear combination of the matrices I and J, $U_j = \omega I + \tau J$, where $\omega, \tau \in \mathbb{C}$. Using the relation (2.4) one obtains

$$J - i\alpha_j I = (J + i\alpha_j I)(\omega I + \tau J) = i\alpha_j\omega I + (\omega + i\alpha_j\tau + d_j\tau)J\,.$$

The comparison of the corresponding terms gives

$$\omega = -1\,, \quad \tau = \frac{2}{d_j + i\alpha_j}\,, \quad U_j = \frac{2}{d_j + i\alpha_j} J - I\,. \tag{2.5}$$

The case with $\alpha_j = 0$ corresponds to the so-called *free boundary conditions*; some authors also call them Kirchhoff or Neumann. The case $\alpha_j = \infty$, i. e. $\psi_{jn} = 0$, corresponds to decoupled edges with *Dirichlet boundary conditions*.

2. $\delta'_{\rm s}$-coupling:

$$\begin{aligned} \psi'_j := \psi'_{jn}(j) &= \psi'_{jm}(j) \quad \text{for all } n, m \in \nu(j)\,, \\ \sum_{n\in\nu(j)} \psi_{jn}(j) &= \beta_j \psi'_j \end{aligned}$$

with $\beta_j \in \mathbb{R}$. Similarly to the previous case, we choose $A_j = J$, $B_j = -\beta_j I$, $U_j = \omega I + \tau J$. The relation (2.3) gives

$$J + i\beta_j I = (-J + i\beta_j I)(\omega I + \tau J) = i\beta_j \omega I + (i\beta_j \tau - d_j \tau - \omega) J\,,$$

while the comparison of the corresponding terms gives

$$\omega = 1\,, \quad \tau = -\frac{2}{d_j - i\beta_j}\,, \quad U_j = I - \frac{2}{d_j - i\beta_j} J\,.$$

The particular case $\beta_j = \infty$ corresponds again to decoupled edges, this time with *Neumann boundary conditions*.

3. δ'-coupling:

$$\begin{aligned} \psi_{jn}(j) - \psi_{jm}(j) &= \frac{\beta_j}{d_j}[\psi'_{jn}(j) - \psi'_{jm}(j)] \quad \text{for all } n, m \in \nu(j)\,, \\ \sum_{n\in\nu(j)} \psi'_{jn}(j) &= 0 \end{aligned}$$

with $\beta_j \in \mathbb{R}$. The matrices can be chosen as $A_j = d_j I - J$, $B_j = -\beta_j I$, $U_j = \omega I + \tau J$. The relation (2.4) gives

$$(-\beta_j + d_j i) I - iJ = [(-\beta_j - i d_j) I + iJ](\omega I + \tau J)\,,$$

while the comparison of the corresponding terms gives

$$\omega = -\frac{d_j + i\beta_j}{d_j - i\beta_j}\,, \quad \tau = \frac{2}{d_j - i\beta_j}\,, \quad U_j = \frac{2}{d_j - i\beta_j} J - \frac{d_j + i\beta_j}{d_j - i\beta_j} I\,.$$

2.3 Exterior complex scaling

In dealing with resonances, the approach first introduced by Aguilar and Combes in [AC71] is useful. Since the resonances cannot be described as the eigenvalues of a self-adjoint operator, one performs a complex coordinate change and obtains an equivalent operator. However, the new operator is not self-adjoint and the resonances correspond to its complex eigenvalues.

To be specific, we consider a scaling transformation on all semi-infinite edges $g(x) \to g_\theta(x) = U_\theta g(x) = \mathrm{e}^{\theta/2} g(x\mathrm{e}^\theta)$ with a complex parameter θ, common to all the halflines, while the functions on Γ_e stay unchanged.

We may demonstrate the transformation of the free motion Hamiltonian on a halfline by the action on a function g.

$$H_\theta g(x) = U_\theta H U_\theta^{-1} g(x) = U_\theta H \mathrm{e}^{-\theta/2} g(x\mathrm{e}^{-\theta}) = -\mathrm{e}^{-\theta/2} U_\theta [g(x\mathrm{e}^{-\theta})]'' = \\ = -\mathrm{e}^{-\theta/2}\mathrm{e}^{-2\theta} U_\theta g''(x\mathrm{e}^{-\theta}) = -\mathrm{e}^{-\theta/2}\mathrm{e}^{\theta/2}\mathrm{e}^{-2\theta} g''(x) = \mathrm{e}^{-2\theta} H g(x).$$

This means that the Hamiltonian is transformed by multiplying by $\mathrm{e}^{-2\theta}$ on the halfline, and this leads to the corresponding change of the boundary conditions which consists of adding the factor $\mathrm{e}^{-2\theta}$ at appropriate places.

Let us consider the Hamiltonian on a graph Γ_e acting as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ on the external links and as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_{jn}(x)$ on $\mathcal{L}_{jn}$ where V_{jn} is assumed to be essentially bounded. We use the mentioned transformation on the external edges. The transformed Hamiltonian is

$$H_\theta \begin{pmatrix} \{g_j\} \\ \{f_{jn}\} \end{pmatrix} = \begin{pmatrix} \{-\mathrm{e}^{-2\theta} g_j''\} \\ \{-f_{jn}'' + V_{jn} f_{jn}\} \end{pmatrix}$$

where g_j is the wavefunction on the halfline attached to the point $\mathcal{X}_j$ and f_{jn} the wavefunction on $\mathcal{L}_{jn}$, similarly for other edges of the graph: the sets $\{g_j\}$ and $\{f_{jn}\}$ refer to all external links and internal edges, respectively. The domain of definition of the transformed Hamiltonian consists of functions with components $f_{jn} \in W^{2,2}([0, l_{jn}])$ and $g_{j\theta} = U_\theta g_j$ satisfying the coupling conditions.

Furthermore, we are interested in the situation, when the imaginary part of θ is nontrivial; without loss of generality we may choose $\theta = i\vartheta$ with $\vartheta \in \mathbb{R}_+$. Then the essential spectrum of the Hamiltonian rotates into the lower complex plain. If ϑ is large enough we can reveal the resonance poles in the second sheet of the Riemann surface of energy.

2.4 Attaching more semiinfinite links to one vertex

Now we can use the method introduced in the previous section for obtaining a set of equations for poles of the resolvent of the Hamiltonian. In this section we slightly generalize the problem studied in [EL06]. Let us consider a vertex of the graph to which M semiinfinite external links and N internal links are attached. Let us suppose separate δ-coupling at each bundle and following coupling between bundles (as in [E97b])

$$f_1(0) = \cdots = f_N(0) =: f(0)\,, \quad g_1(0) = \cdots = g_M(0) =: g(0)\,, \tag{2.6}$$

$$f(0) \;=\; \alpha^{-1} \sum_{n=1}^{N} f_n'(0) + \gamma \sum_{m=1}^{M} g_m'(0)\,, \tag{2.7}$$

$$g(0) \;=\; \bar\gamma \sum_{n=1}^{N} f_n'(0) + \tilde\alpha^{-1} \sum_{m=1}^{M} g_m'(0)\,. \tag{2.8}$$

Performing the complex scaling of the semiinfinite links one can obtain

$$f(0) = \alpha^{-1} \sum_{n=1}^{N} f_n'(0) + \gamma ikM \mathrm{e}^{-3\theta/2}\mathrm{e}^{\theta}\, g_\theta(0)\,,$$

$$\mathrm{e}^{-\theta/2} g_\theta(0) = \bar\gamma \sum_{n=1}^{N} f_n'(0) + \tilde\alpha^{-1} ikM \mathrm{e}^{-\theta/2} g_\theta(0)\,.$$

Expressing $\mathrm{e}^{-\theta/2} g_\theta(0)$ from the last equation and substituting it into the other one we obtain an equation formally similar to the δ-coupling,

$$f(0) = \left(\alpha^{-1} + \frac{|\gamma|^2 ikM}{1 - ik\tilde\alpha^{-1}M}\right) \sum_{n=1}^{N} f_n'(0)\,.$$

We denote by $\beta(k)$ the effective energy dependent coupling parameter

$$\beta^{-1}(k) = \alpha^{-1} + \frac{|\gamma|^2 ikM}{1 - ik\tilde\alpha^{-1}M} \quad \Rightarrow \quad \beta(k) = \alpha \frac{1 - ikM\tilde\alpha^{-1}}{1 + ikM\,(|\gamma|^2\alpha - \tilde\alpha^{-1})}\,. \tag{2.9}$$

The parameter γ controls the coupling, choosing $|\gamma| = 0$ we can disconnect the bundle of semiinfinite links. The considered coupling also includes the overall δ-coupling of all the involved links; choosing $\alpha = \tilde\alpha = \gamma^{-1}$ the effective coupling constant becomes $\beta(k) = \alpha - ikM$.

Effectively, the quantum graph with attached semiinfinite links Γ can be thus replaced by the corresponding finite graph Γ_e with new non-selfadjoint energy dependent coupling

$$f_{jn}(j) =: f_j(j), \quad \forall n \in \nu(j)\,, \tag{2.10}$$

$$f_j(j) = \beta_j^{-1}(k) \sum_{n\in\nu(j)} f'_{jn}(j)\,. \tag{2.11}$$

at the "outer" vertices. For vertices $j \notin I_{\mathcal{C}}$ we simply assume $\beta_j(k) = \alpha_j$.

2.5 Equivalence of the resolvent and scattering resonances on a quantum graph

We can use the result of previous section to show that the resolvent and scattering resonances coincide. Let us think of the quantum graph Γ_e as the scattering center and of the semiinfinite links as the incoming and outgoing wires. The scattering matrix (S-matrix) maps the vector of the amplitudes of the incoming waves to the vector of the amplitudes of the outgoing waves. From the coupling condition we obtain a set of equations for the coefficients of the incoming and outgoing waves. The poles of the S-matrix are given by the condition $\det S^{-1} = 0$.

Using the duality between the Hamiltonian on quantum graph and a certain Jacobi-type matrix (theorem 3.1 in [E97a]) we obtain from (2.10) – (2.11) the set of equations which involve only the functional values at the vertices. A comparison of both systems of equation gives following theorem. It slightly generalizes the theorem 3.2 in [EL06], obtained only for graphs where at most one semiinfinite link was attached to every vertex of the graph.

Theorem 2.1. *Let Γ be a quantum graph with one or more semiinfinite links attached to some vertices. We assume the coupling conditions at the vertices from $\mathcal{C}$ are (2.6) – (2.8) and δ-conditions at the other vertices. Then the families of its resolvent and scattering resonances coincide.*

Proof. The proof is formally identical to the proof of the theorem 3.2 in [EL06]. One must only realize that the effective coupling constant $\beta(k)$ is given by a different term (2.9). □

With the previous theorem in mind, we are no longer forced to distinguish between the poles of the S-matrix and the poles of the resolvent of the Hamiltonian above. Therefore, we can use the method of the external complex scaling in the next chapter to determine the resonance poles.

Chapter 3

Resonances from perturbations of the graphs with rational rate of lengths of the edges

In this chapter, we will study the spectrum of a quantum graph with rational rate of lengths of some its edges and its behaviour in the case when the lengths of the edges are perturbed.

If a quantum graph contains some edges with rational rate of their lengths then eigenvalues (their square roots are multiples of π/l) may occur embedded into its continuous spectrum. In particular, we prove that these eigenvalues are present in the spectrum of a graph with a closed loop of edges with rational rate of their lengths or a graph containing a line segment of edges with rational rate of their lengths with Dirichlet or Neumann conditions at both ends of the segment. The eigenfunctions corresponding to these eigenvalues are $\sin kx$ (or $\cos kx$ for Neumann conditions) with zeros in the vertices of the loop or line and they vanish outside the considered loop or line. The spectrum may contain eigenvalues embedded in the continuous, with the eigenfunctions which vanish at the vertices. They are multiples of $(\pi/l)^2$ where l is the length "unit".

When changing the ratio of the lengths of the edges, the poles of the resolvent (formerly corresponding to the eigenvalues) become resonances. In the following two simple examples we investigate trajectories of the resonances depending on the lengths of the edges and other properties of the spectrum. As the main result, we prove afterwards that an embedded eigen-

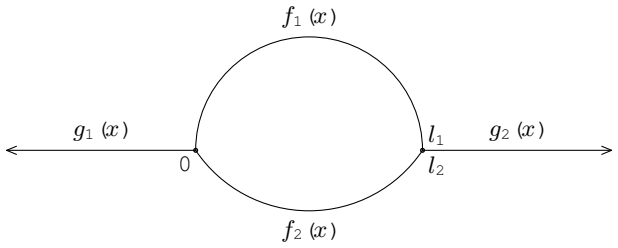

Figure 3.1: A loop with two leads

value of multiplicity n gives rise to n resonances in the spectrum of the perturbed graph.

3.1 A loop with two leads

Let us consider the graph on figure 3.1 consisting of two internal edges of lengths l_1, l_2, one halfline is connected to each endpoint. The Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$ on each link. The corresponding Hilbert space is $L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^+) \oplus L^2([0,l_1]) \oplus L^2([0,l_2])$; states are described by columns $\psi = (g_1, g_2, f_1, f_2)^T$. Let us consider the following coupling conditions corresponding to more general case discussed in section 2.4.

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

Using the method of external complex scaling $g_{i\theta}(x) = \mathrm{e}^{\theta/2} g_i(x\mathrm{e}^{\theta})$ introduced in the section 2.3 and the Ansatz $f_i(x) = a_i \sin kx + b_i \cos kx$, $i = 1, 2$

we obtain

$$\begin{aligned}
b_1 &= b_2\,,\\
a_1\sin kl_1 + b_1\cos kl_1 &= a_2\sin kl_2 + b_2\cos kl_2\,,\\
b_1 &= \alpha_1^{-1}k(a_1+a_2) + \gamma_1 ik\mathrm{e}^{-\theta/2}g_{1\theta}(0)\,,\\
a_1\sin kl_1 + b_1\cos kl_1 &= -\alpha_2^{-1}k(a_1\cos kl_1 - b_1\sin kl_1 + a_2\cos kl_2 - b_2\sin kl_2)\\
&\qquad + \gamma_2 ik\mathrm{e}^{-\theta/2}g_{2\theta}(0)\,,\\
\mathrm{e}^{-\theta/2}g_{1\theta}(0) &= \bar\gamma_1 k(a_1+a_2) + \tilde\alpha_1^{-1}ik\mathrm{e}^{-\theta/2}g_{1\theta}(0)\,,\\
\mathrm{e}^{-\theta/2}g_{2\theta}(0) &= -\bar\gamma_2 k(a_1\cos kl_1 - b_1\sin kl_1 + a_2\cos kl_2 - b_2\sin kl_2)\\
&\qquad + \tilde\alpha_2^{-1}ik\mathrm{e}^{-\theta/2}g_{2\theta}(0)\,.
\end{aligned}$$

The condition of solvability of this system is

$$\begin{vmatrix}
0 & 1 & 0 & -1\\
\sin kl_1 & \cos kl_1 & -\sin kl_2 & -\cos kl_2\\
-k\beta_1^{-1} & 1 & -k\beta_1^{-1} & 0\\
\sin kl_1 + k\beta_2^{-1}\cos kl_1 & \cos kl_1 - k\beta_2^{-1}\sin kl_1 & k\beta_2^{-1}\cos kl_2 & -k\beta_2^{-1}\sin kl_2
\end{vmatrix} = 0\,,$$

where

$$\beta_j^{-1}(k) = \alpha_j^{-1} + \frac{ik|\gamma_j|^2}{1-ik\tilde\alpha_j^{-1}} = \alpha_j^{-1} - \frac{k^2|\gamma_j|^2\tilde\alpha_j^{-1}}{1+k^2\tilde\alpha_j^{-2}} + \frac{ik|\gamma_j|^2}{1+k^2\tilde\alpha_j^{-2}}\,. \qquad (3.1)$$

After a simple algebra we obtain the final condition

$$\begin{aligned}
&\sin kl_1\sin kl_2 - 4k^2\beta_1^{-1}(k)\beta_2^{-1}(k)\sin^2\left(k\frac{l_1+l_2}{2}\right) +\\
&\qquad + k[\beta_1^{-1}(k)+\beta_2^{-1}(k)]\sin k(l_1+l_2) = 0\,.
\end{aligned}$$

We parametrize the length of the edges by the parameter λ as follows

$$l_1 = l(1-\lambda)\,,\quad l_2 = l(1+\lambda)\,,$$

then the condition becomes

$$\begin{aligned}
&\sin kl(1-\lambda)\sin kl(1+\lambda) - 4k^2\beta_1^{-1}(k)\beta_2^{-1}(k)\sin^2 kl +\\
&\qquad + k[\beta_1^{-1}(k)+\beta_2^{-1}(k)]\sin 2kl = 0\,. \qquad (3.2)
\end{aligned}$$

Let us compute the difference of the first terms in (3.2) for different λ, λ'. Using trigonometrical identities we get

$$\begin{aligned}\sin kl(1-\lambda')\sin kl(1+\lambda') - \sin kl(1-\lambda)\sin kl(1+\lambda) = \\ = \frac{1}{2}[\cos 2\lambda' kl - \cos 2kl - \cos 2\lambda kl + \cos 2kl] = \\ = -\sin kl(\lambda+\lambda')\sin kl(\lambda'-\lambda) = -\sin kl(2\lambda+\varepsilon)\sin kl\varepsilon\,.\end{aligned}$$

We have denoted here the difference $\lambda' - \lambda$ by ε. Hence if k_0 is the solution of (3.2) for parameter λ then the solution k for parameter λ' satisfies the equation

$$\begin{aligned}\sin kl(1-\lambda)\sin kl(1+\lambda) - 4k^2\beta_1^{-1}(k)\beta_2^{-1}(k)\sin^2 kl + \\ + k[\beta_1^{-1}(k) + \beta_2^{-1}(k)]\sin 2kl = \sin kl(2\lambda+\varepsilon)\sin kl\varepsilon\,.\end{aligned}$$

Let us suppose that k depends on ε continuously. If the difference $k_1 = k - k_0$ is small we obtain using the Taylor expansion

$$\begin{aligned}k_1 l[\sin(2k_0 l) - \lambda\sin(2k_0 l\lambda)] - 4k_1 l k_0^2\beta_1^{-1}(k_0)\beta_2^{-1}(k_0)\sin 2k_0 l - \\ - 4k_1[2k_0\beta_1^{-1}(k_0)\beta_2^{-1}(k_0) + k_0^2(\beta_1^{-1}(k_0)\tilde\beta_2(k_0) + \tilde\beta_1(k_0)\beta_2^{-1}(k_0))]\sin^2 k_0 l + \\ + k_1(\beta_1^{-1}(k_0) + \beta_2^{-1}(k_0) + \tilde\beta_1(k_0)k_0 + \tilde\beta_2(k_0)k_0)\sin 2k_0 l + 2k_1 l k_0(\beta_1^{-1}(k_0) + \\ + \beta_2^{-1}(k_0))\cos 2k_0 l - k_1 l[\varepsilon\cos k_0 l\varepsilon\sin k_0 l(2\lambda+\varepsilon) + \\ + (2\lambda+\varepsilon)\cos k_0 l(2\lambda+\varepsilon)\sin k_0 l\varepsilon] + \mathcal{O}(k_1^2) = \sin k_0 l(2\lambda+\varepsilon)\sin k_0 l\varepsilon\,,\end{aligned} \tag{3.3}$$

where $\tilde\beta_j(k_0) = i|\gamma_j|^2/(1 - ik_0\tilde\alpha_j^{-1})^2$.

We can use the previous equation for obtaining k_1. Denoting the coefficient by k_1 by $f(k_0)$ and the rhs of previous equation by $g(\lambda,\varepsilon)$ we have for the error

$$\delta = \frac{\mathcal{O}(k_1^2)}{f(k_0)} = \frac{1}{f(k_0)}\,\mathcal{O}\left(\frac{g^2(\lambda,\varepsilon)}{f^2(k_0,\varepsilon)}\right).$$

Since the rhs of (3.3) is $\mathcal{O}(\varepsilon)$, the error we make by neglecting the term $\mathcal{O}(k_1^2)$ is $\mathcal{O}(\varepsilon^2)$, for $2\lambda k_0 l$ close to $= 2n\pi$ is the error even smaller ($\mathcal{O}(\varepsilon^4)$). Moreover, the trajectories of the resonances obtained numerically can be verified for $\lambda = \frac{m}{n}$ when the embedded eigenvalues given by $kl = n\pi$ are present. The figure 3.6 shows that the resonance poles obtained by direct numerical solving of the equation (3.2) correspond to the ones obtained by solving (3.3).

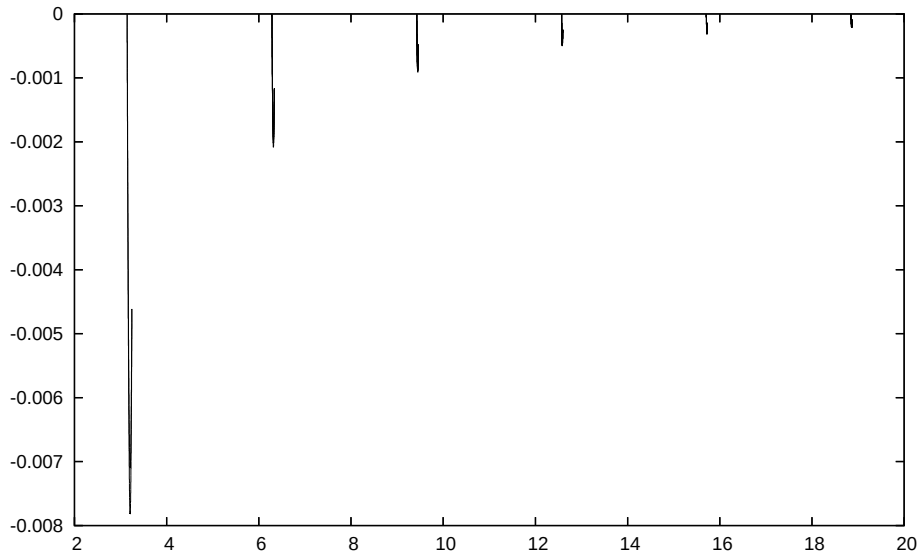

Figure 3.2: The trajectories of several resonance poles (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha_1^{-1} = 1$, $\tilde{\alpha}_1^{-1} = -2$, $|\gamma_1|^2 = 1$, $\alpha_2^{-1} = 1$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_2|^2 = 1$, $n = 1,\ 2,\ 3,\ 4,\ 5,\ 6$.

Therefore, the equation (3.3) can be used for numerical computation of the pole trajectories on figures 3.2 – 3.5. The change of the parameter λ from 0 to 1 is represented by changing the colour from red ($\lambda = 0$) to blue ($\lambda = 1$). On figures 3.7 – 3.12 the dependence of the length of the curve and its change (velocity) on the parameter λ is plotted.

The equation (3.2) has real solution $kl = n\pi$, $n \in \mathbb{N}$ for $\lambda = m/n$, $m \in \mathbb{N}$. The corresponding eigenfunction is $\psi = (0, 0, \sin n\pi x/l, -\sin n\pi x/l)^T$. On the figure 3.3 ($n = 2$) the pole returns to the real axis if $\lambda = 1/2$ and $\lambda = 1$. On figure 3.4 ($n = 3$) the pole returns to the real axis only for $\lambda = 2/3$. For $\lambda = 1/3$ and $\lambda = 1$ the appropriate solution is a resonance. Similarly, on figure 3.5 ($n = 2$) the pole returns to the real axis only for $\lambda = 1$.

The condition (3.2) can be rewritten as

$$f(k,\lambda) = \cos 2kl\lambda - \cos 2kl - 8k^2\beta_1^{-1}(k)\beta_2^{-1}(k)\sin^2 kl + \\ + 2k(\beta_1^{-1}(k) + \beta_2^{-1}(k))\sin 2kl = 0\,. \quad (3.4)$$

Let us investigate the asymptotic behaviour of the resonances for small ε, in particular, the angle φ between the pole trajectory going from $k_0 = n\pi/l$

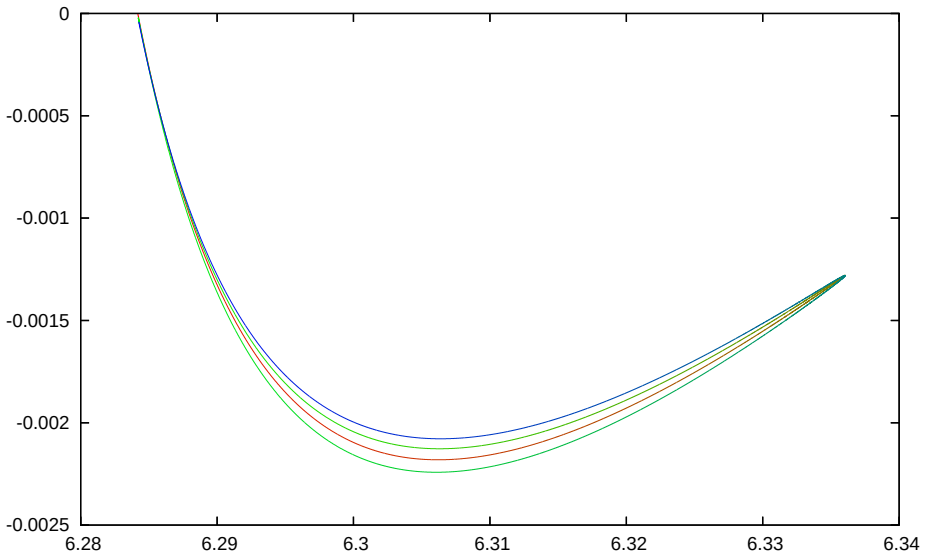

Figure 3.3: The trajectory of the resonance pole $k_0 = 2\pi$ (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha_1^{-1} = 1$, $\tilde{\alpha}_1^{-1} = -2$, $|\gamma_1|^2 = 1$, $\alpha_2^{-1} = 0$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_2|^2 = 1$, $n = 2$. The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

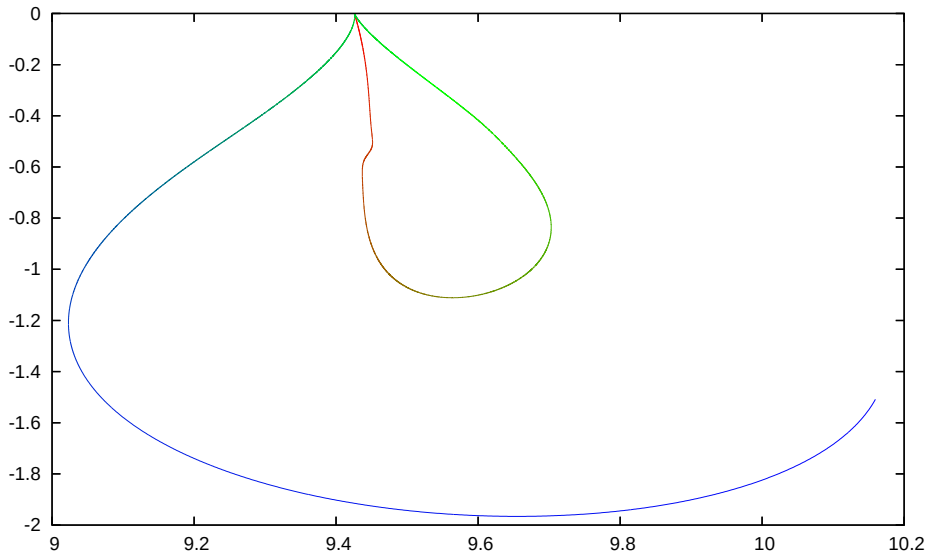

Figure 3.4: The trajectory of the resonance pole $k_0 = 3\pi$ (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha_1^{-1} = 1$, $\alpha_2^{-1} = 1$, $\tilde{\alpha}_1^{-1} = 1$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_1|^2 = |\gamma_2|^2 = 1$, $n = 3$. The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

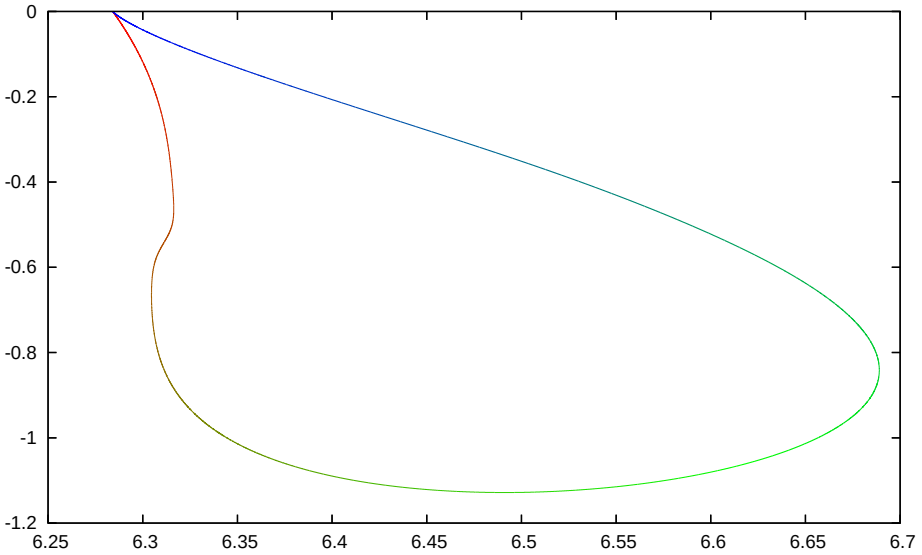

Figure 3.5: The trajectory of the resonance pole $k_0 = 2\pi$ (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha_1^{-1} = 1$, $\alpha_2^{-1} = 1$, $\tilde{\alpha}_1^{-1} = 1$, $\tilde{\alpha}_2^{-1} = 1$, $|\gamma_1|^2 = 1$, $|\gamma_2|^2 = 1$, $n = 2$. The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

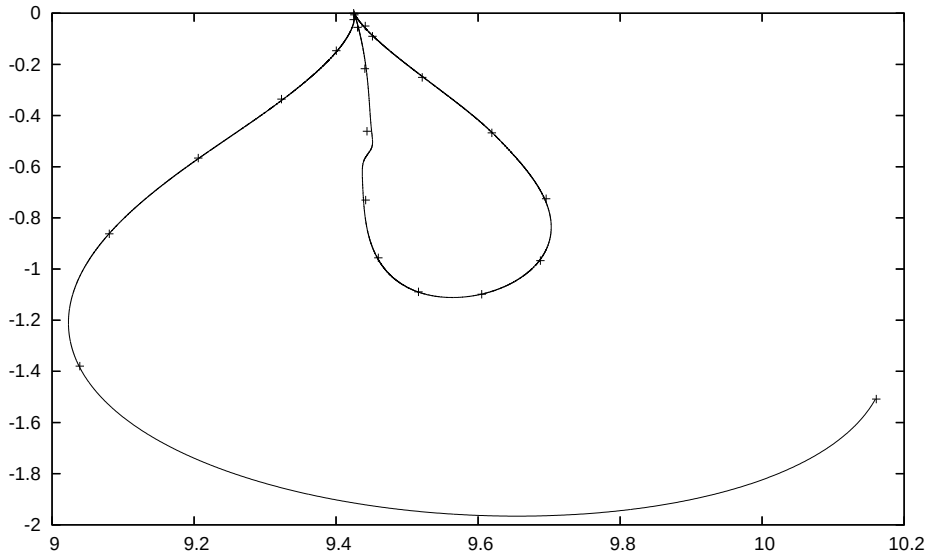

Figure 3.6: A comparison of the trajectory of the resonance pole from the figure 3.4 obtained from the equation (3.3) – the full line – and the resonance poles obtained by numerical solving of the equation (3.2) for λ equal to multiples of 0.05 (represented by crosses). It shows that the error we make by using the approximate equation (3.3) is small (for $\lambda = 0.2$ approximately $6 \cdot 10^{-3}$).

with $\lambda_0 = m/n, m \in \{0, 1, \dots, n\}$ and the horizontal line. For small k_1 the difference $\varepsilon = \lambda - \lambda_0$ is also small. The function $f(k, \lambda)$ is with the exception of points $k = -i\tilde{\alpha}_j$ continuous and its first partial derivative with respect to λ is at λ_0 equal to zero. Hence

$$
\begin{aligned}
0 = f(k,\lambda) \approx f(k_0,\lambda_0) + \left.\frac{\partial^2 f}{\partial \lambda^2}\right|_{k_0,\lambda_0} \varepsilon^2 + \left.\frac{\partial f}{\partial k}\right|_{k_0,\lambda_0} k_1 \,. \\
\left.\frac{\partial f}{\partial k}\right|_{k_0,\lambda_0} = 4n\pi \left[\beta_1^{-1}(k_0) + \beta_2^{-1}(k_0)\right] \,, \\
\left.\frac{\partial^2 f}{\partial \lambda^2}\right|_{k_0,\lambda_0} = -4(kl)^2 \cos 2kl\lambda = -4(\pi n)^2 \,.
\end{aligned}
$$

For small k_1 we obtain using (3.1)

$$
\begin{aligned}
k_1 \approx \varepsilon^2 \frac{\pi n}{\beta_1^{-1}(k_0) + \beta_2^{-1}(k_0)} \,, \\
\tan\varphi = \frac{\operatorname{Im} k_1}{\operatorname{Re} k_1} = \frac{\frac{k_0|\gamma_1|^2}{1+k_0^2\tilde{\alpha}_1^{-2}} + \frac{k_0|\gamma_2|^2}{1+k_0^2\tilde{\alpha}_2^{-2}}}{\alpha_1^{-1} + \alpha_2^{-1} - \frac{k_0^2|\gamma_1|^2\tilde{\alpha}_1^{-1}}{1+k_0^2\tilde{\alpha}_1^{-2}} - \frac{k_0^2|\gamma_2|^2\tilde{\alpha}_2^{-1}}{1+k_0^2\tilde{\alpha}_2^{-2}}} \,, \quad k_0 = \frac{n\pi}{l} \,. \qquad (3.5)
\end{aligned}
$$

For $|\gamma_1| = |\gamma_2| = 0$ the poles are real and $\varphi = 0$. Otherwise, if $\alpha_1^{-1} = \tilde{\alpha}_1^{-1} = \alpha_2^{-1} = \tilde{\alpha}_2^{-1} = 0$ then the real part of k_1 is zero and the pole trajectory goes from k_0 perpendicular to the horizontal line ($\varphi = \pi/2$).

Further, let us investigate the behavior of the pole trajectories for big n. Let us suppose that $k = k_0 + k_1$, $k_0 = n\pi/l$, $|k_1| \ll \pi/l$. Then

$$
\begin{aligned}
\cos 2kl\lambda - \cos 2kl = \cos 2k_0 l\lambda \cos 2k_1 l\lambda - \sin 2k_0 l\lambda \sin 2k_1 l\lambda - \cos 2k_1 l = \\
= (\cos 2n\pi\lambda - 1) - \sin(2\pi n\lambda)\, 2k_1 l\lambda + \mathcal{O}(k_1^2) \,.
\end{aligned}
$$

The condition (3.4) for small k_1 becomes

$$
\begin{aligned}
(\cos 2n\pi\lambda - 1) - \sin(2\pi n\lambda)\, 2k_1 l\lambda + \\
+ 2\frac{n\pi}{l}\left[\beta_1^{-1}(k_0) + \beta_2^{-1}(k_0)\right] 2k_1 l + \mathcal{O}(k_1^2) = 0 \,.
\end{aligned}
$$

From (3.1) we obtain

$$
\begin{aligned}
\beta_j^{-1}(k_0) = \alpha_j^{-1} - \frac{|\gamma_j|^2}{\tilde{\alpha}_j^{-1}} + i\frac{l|\gamma_j|^2}{n\pi\tilde{\alpha}_j^{-2}} + \mathcal{O}\left(\frac{1}{n^2}\right), \qquad \text{for} \quad \tilde{\alpha}_j^{-1} \neq 0 \,, \\
\beta_j^{-1}(k_0) = i\frac{n\pi}{l}|\gamma_j|^2 + \mathcal{O}(1), \qquad \text{for} \quad \tilde{\alpha}_j^{-1} = 0 \,.
\end{aligned}
$$

The functions

$$|\cos(2n\pi\lambda) - 1| \le 2\,, \quad |\sin(2\pi k_1 l\lambda)| \le 1$$

are bounded, therefore for $\tilde{\alpha}_1^{-1} \neq 0$, $\tilde{\alpha}_2^{-1} \neq 0$ we have

$$|\mathrm{Im}\, k_1| \le \frac{l}{2(\pi n)^2} \frac{|\gamma_1|^2/\tilde{\alpha}_1^{-2} + |\gamma_2|^2/\tilde{\alpha}_2^{-2}}{(\alpha_1^{-1} + \alpha_2^{-1} - |\gamma_1|^2/\tilde{\alpha}_1^{-1} - |\gamma_2|^2/\tilde{\alpha}_2^{-1})^2} + \mathcal{O}\left(\frac{1}{n^3}\right)\,,$$

while for $\tilde{\alpha}_1^{-1} = 0$, $\tilde{\alpha}_2^{-1} = 0$ the inequality reads

$$|\mathrm{Im}\, k_1| \le \frac{l}{2(\pi n)^2} \frac{1}{|\gamma_1|^2 + |\gamma_2|^2} + \mathcal{O}\left(\frac{1}{n^3}\right)\,,$$

and for $\tilde{\alpha}_1^{-1} = 0$, $\tilde{\alpha}_2^{-1} \neq 0$ we have

$$|\mathcal{I}m\, k_1| \le \frac{l}{2(\pi n)^2} \frac{1}{|\gamma_1|^2} + \mathcal{O}\left(\frac{1}{n^3}\right)\,.$$

Let us summarize our results. The poles of the resolvent are given by the condition (3.2) or its equivalent (3.4). For $\lambda = m/n$, $m \in \mathbb{N}$ real eigenvalues $kl = n\pi$, $n \in \mathbb{N}$ occur. They may correspond to one pole of the resolvent returning to the real axis for $\lambda = m/n$, $m \in \mathbb{N}$ as in figure 3.3. However, for other combinations of the coupling conditions, the pole may return only for certain λ (see figures 3.4 and 3.5). For other rational λ, its place is taken by the pole which has been resonance for $\lambda = 0$. The angle between the trajectory of the resonance and the real axis does not depend on λ and is given by (3.5). If the trajectory of the pole is near the original eigenvalue then the distance from the real axis is of order $\mathcal{O}(1/n^2)$ for big n. This behaviour can be seen, e. g., on figure 3.2. It is also interesting to investigate the velocity (i. e. the term $|k_1|/\varepsilon$) and the length of the curve depending on λ on figures (3.7) – (3.12). We can notice that on figure (3.7) the velocity is nonzero but rather small at the right endpoint of the curve.

3.2 A cross-shaped resonator

We consider a graph consisting of two leads and two internal edges attached to the leads at one point (see picture 3.13). The lengths of the internal edges are $l_1 = l(1-\lambda)$ and $l_2 = l(1+\lambda)$. The Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$. The corresponding Hilbert space is $L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^+) \oplus L^2([0,l_1]) \oplus L^2([0,l_2])$,

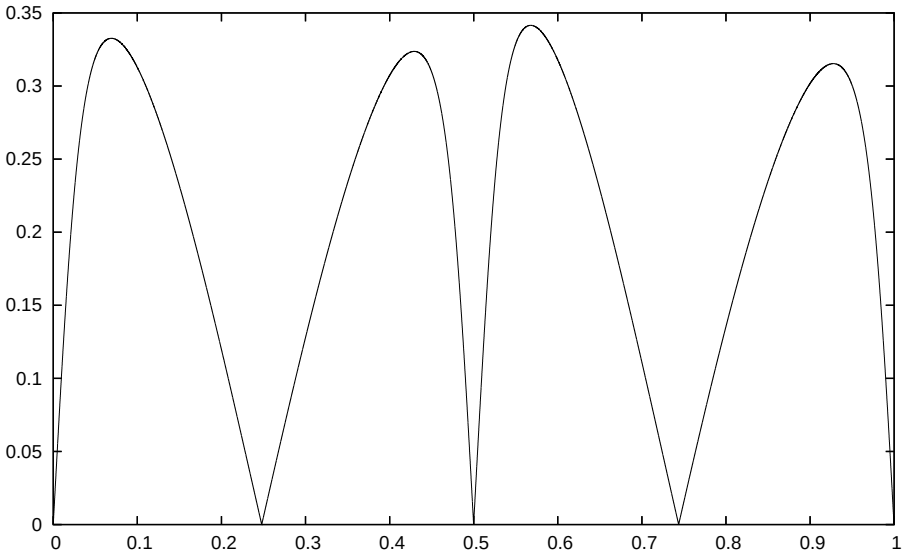

Figure 3.7: The "velocity" (the derivative of the length of the curve with respect to the ratio λ) depending on λ for Figure 3.3.

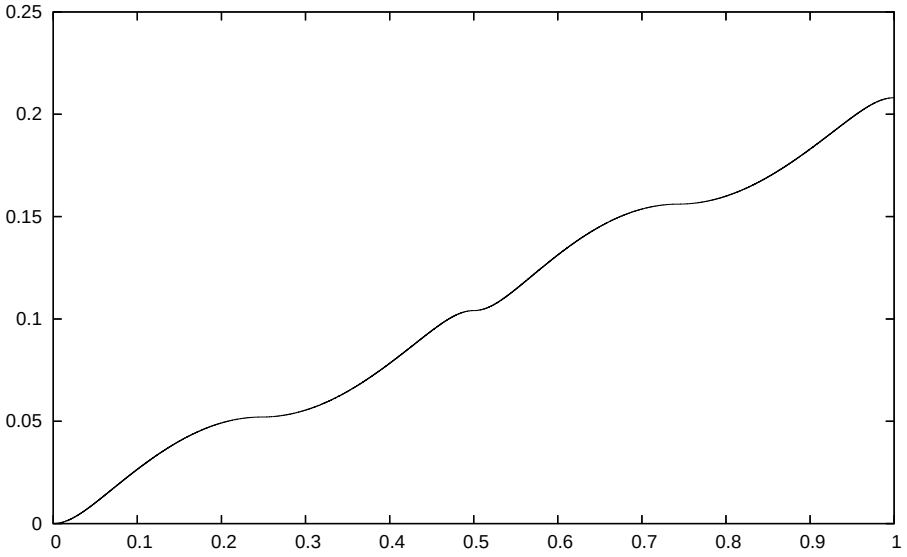

Figure 3.8: The length of the curve depending on λ for Figure 3.3.

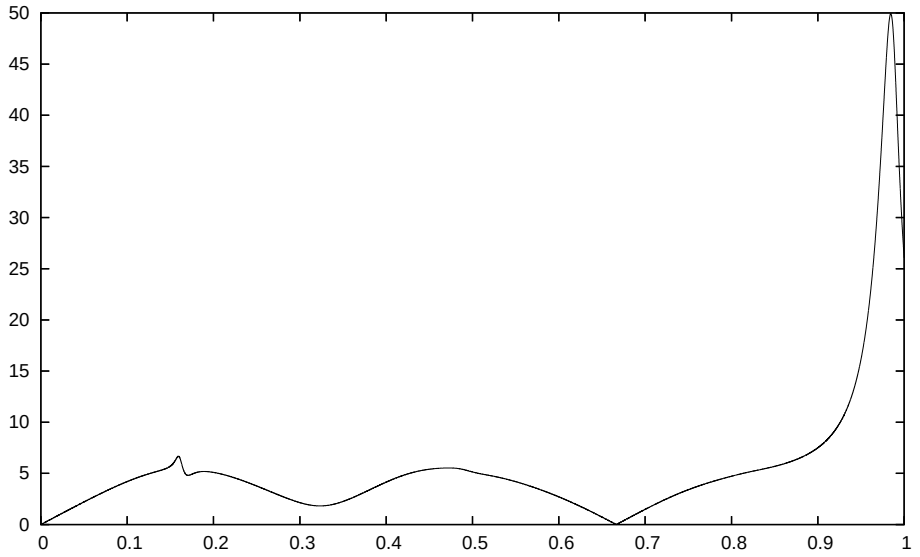

Figure 3.9: The "velocity" (the derivative of the length of the curve with respect to the ratio λ) depending on λ for Figure 3.4.

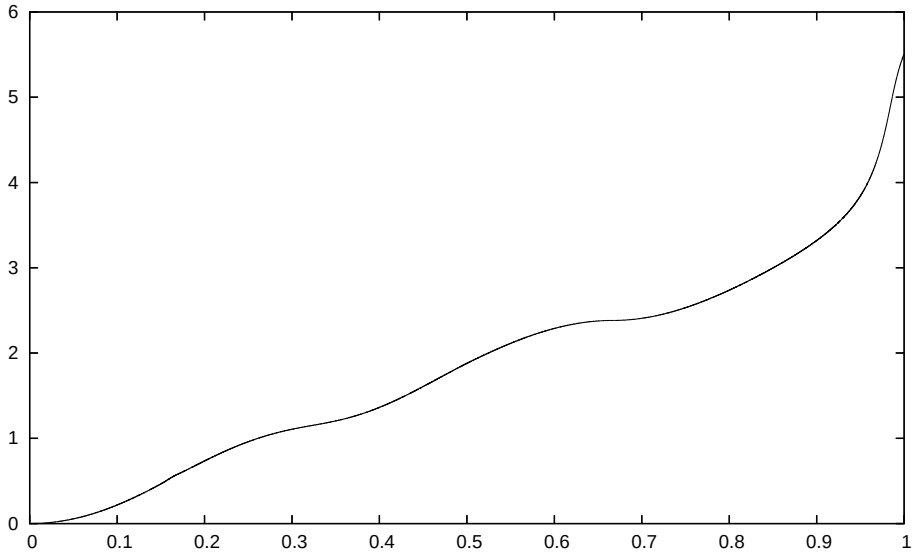

Figure 3.10: The length of the curve depending on λ for Figure 3.4.

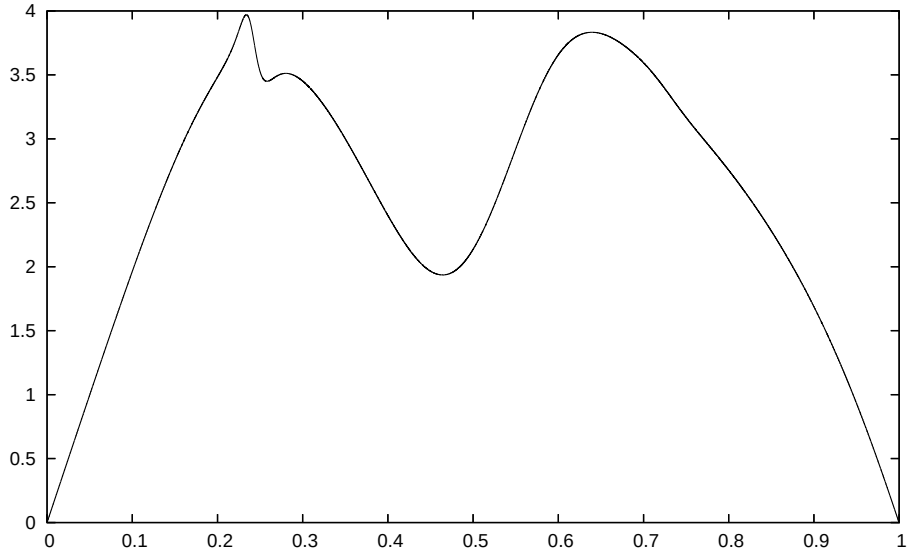

Figure 3.11: The "velocity" (the derivative of the length of the curve with respect to the ratio λ) depending on λ for Figure 3.5.

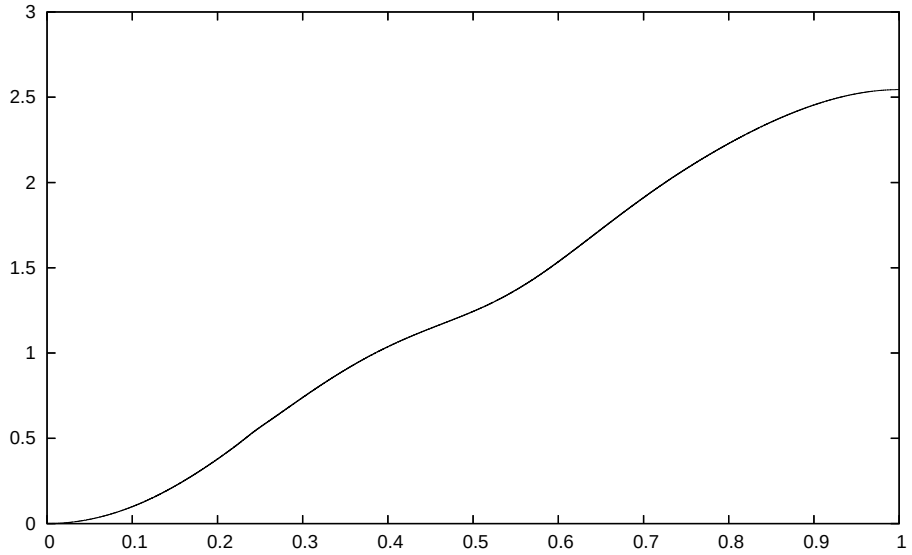

Figure 3.12: The length of the curve depending on λ for Figure 3.5.

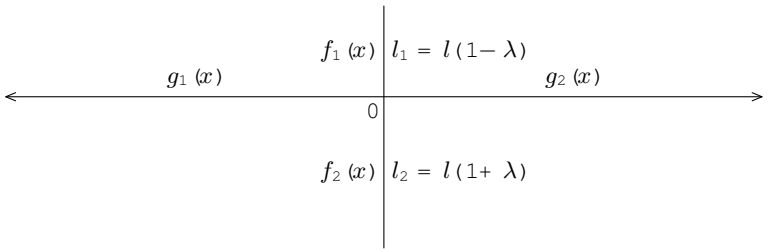

Figure 3.13: A cross-shaped resonator

states are described by columns $\psi = (g_1, g_2, f_1, f_2)^T$. The coupling condition is now a bit simpler, namely

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

Using the method of external complex scaling ($g_{i\theta} = \mathrm{e}^{\theta/2} g_i(x\mathrm{e}^{\theta})$) and the Ansatz $f_i = c_i \sin k(x - l_i)$, $i = 1, 2$ we obtain

$$\begin{aligned} -c_1 \sin(kl_1) &= -c_2 \sin(kl_2) = \mathrm{e}^{-\theta/2} g_\theta(0)\,, \\ -\alpha c_1 \sin kl_1 &= k(c_1 \cos kl_1 + c_2 \cos kl_2) + 2ik\mathrm{e}^{-\theta/2} g_\theta(0)\,. \end{aligned}$$

We choose $c_1 = -c \sin kl_2$, $c_2 = -c \sin kl_1$ and substitute the first equation into the second one.

$$(2ik - \alpha) c \sin kl_1 \sin kl_2 = ck \sin k(l_1 + l_2)\,.$$

Finally, we get two equivalent forms of the condition for resonances

$$\begin{aligned} k \sin 2kl + (\alpha - 2ik) \sin kl(1 - \lambda) \sin kl(1 + \lambda) &= 0\,, \\ 2k \sin 2kl + (\alpha - 2ik)(\cos 2kl\lambda - \cos 2kl) &= 0\,. \end{aligned} \tag{3.6}$$

Let us ask when the solution is real. Leaving out the trivial solution $k = 0$ we get from the last equation two conditions (the real and the imaginary part of the lhs has to be zero)

$$\begin{aligned} \sin 2kl = 0 \quad &\Rightarrow \quad kl = \frac{n\pi}{2}, \quad n \in \mathbb{Z}\,, \\ 0 = \cos 2kl\lambda - \cos 2kl &= \cos n\pi\lambda - \cos n\pi = 2 \sin \frac{n\pi}{2}(1 - \lambda) \sin \frac{n\pi}{2}(1 + \lambda) \\ &\Rightarrow \quad n\lambda = (n - 2m), \quad m \in \mathbb{Z}\,. \end{aligned}$$

Hence $\lambda = 1 - 2m/n$, $m \in \mathbb{N}_0$, $m \leq n/2$.

If the difference $k_1 = k - k_0$ is small we obtain from (3.6)

$$k_1 = -2(\alpha - 2ik_0)\sin k_0 l\varepsilon \sin k_0 l(2\lambda+\varepsilon)/\{2i[\cos 2k_0 l(\lambda+\varepsilon) - \cos 2k_0 l] + (\alpha - 2ik_0)2l[(\lambda+\varepsilon)\sin 2k_0 l(\lambda+\varepsilon) - \sin 2k_0 l] - 2\sin 2k_0 l - 4k_0 l\cos 2k_0 l\}\,. \tag{3.7}$$

Similarly to the previous example, the error is $\mathcal{O}(k_1^2)$, i. e. $\mathcal{O}(\varepsilon^2)$, for $2\lambda k_0 l$ close to $= 2n\pi$ is the error even smaller ($\mathcal{O}(\varepsilon^4)$). Moreover, the trajectories of the resonances received numerically can be again verified for $\lambda = \frac{m}{n}$ when the embedded eigenvalues given by $kl = n\pi$ are present. The figure 3.19 shows that the resonance poles obtained by direct numerical solving of the equation (3.6) correspond to the ones obtained by solving (3.7).

Using the expression above for $k_0 = n\pi/l$, $\lambda = m/n$ and small ε we obtain

$$k_1 = -\frac{2(\alpha - 2ik_0)(k_0 l\varepsilon)^2}{-4k_0 l} = \frac{n\pi\varepsilon^2}{2}\left(\alpha - 2i\frac{n\pi}{l}\right)\,.$$

The angle between the pole trajectory going from k_0 and the horizontal line is

$$\tan\varphi = -\frac{\operatorname{Im} k_1}{\operatorname{Re} k_1} = \frac{2n\pi}{\alpha l} \quad \Rightarrow \quad \varphi = \arctan\frac{2n\pi}{\alpha l}\,. \tag{3.8}$$

The equation (3.6) gives the eigenvalues $kl = n\pi/2$, $n \in \mathbb{Z}$ for $\lambda = 1 - 2m/n$, $m \in \mathbb{N}_0$, $m \leq n/2$. Behaviour of the trajectories of poles is similar to previous example (see figures 3.14–3.20). A pole of the resolvent may return to the same point or it can become another eigenvalue or resonance. An example of the change of the behaviour can be seen on figure 3.20. By a small change of the coupling parameter, parts of the two trajectories can be interchanged (an avoided resonance crossing); The details of the trajectories for different parameters can be seen on figures 3.21 and 3.22. The angle between the trajectory and the real axis is given by (3.8).

3.3 Real eigenvalues for resonator with arbitrary length of the edges

The rational eigenvalues occurred in the previous examples due to Dirichlet boundary conditions in the vertices. In a more general case there are eigenvalues embedded into a continuous spectrum too, but the rationality plays role only for a particular class of coupling conditions.

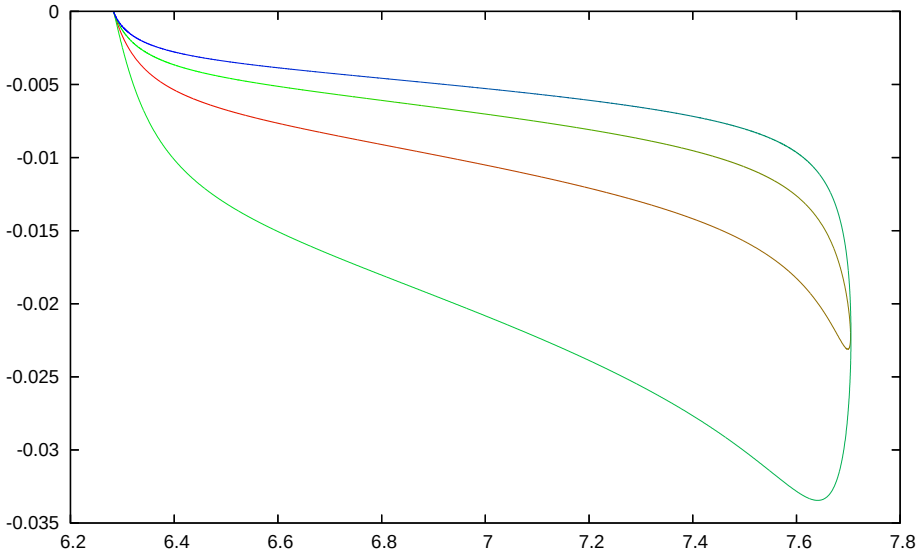

Figure 3.14: The trajectory of the resonance pole $k_0 = 2\pi$ (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha = 100$, $n = 2$. The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

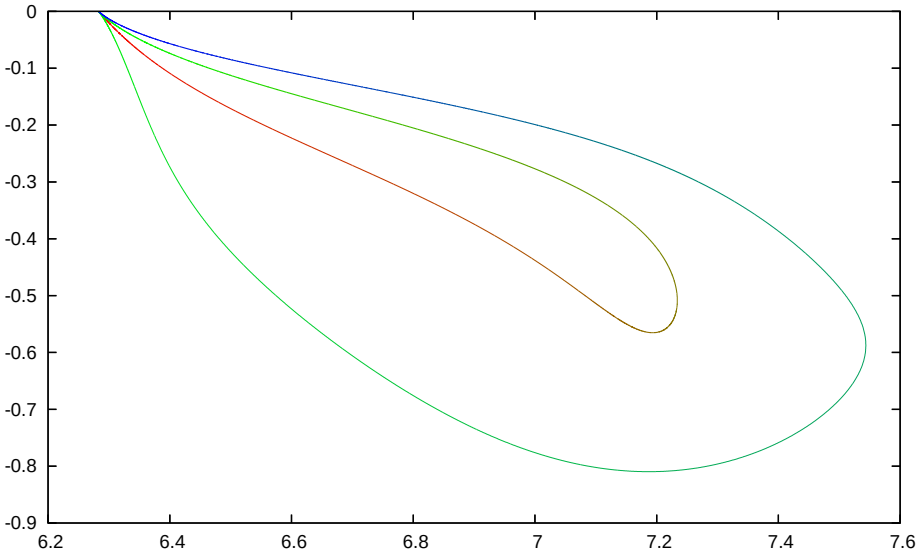

Figure 3.15: The trajectory of the resonance pole $k_0 = 2\pi$ (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha = 10$, $n = 2$. The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

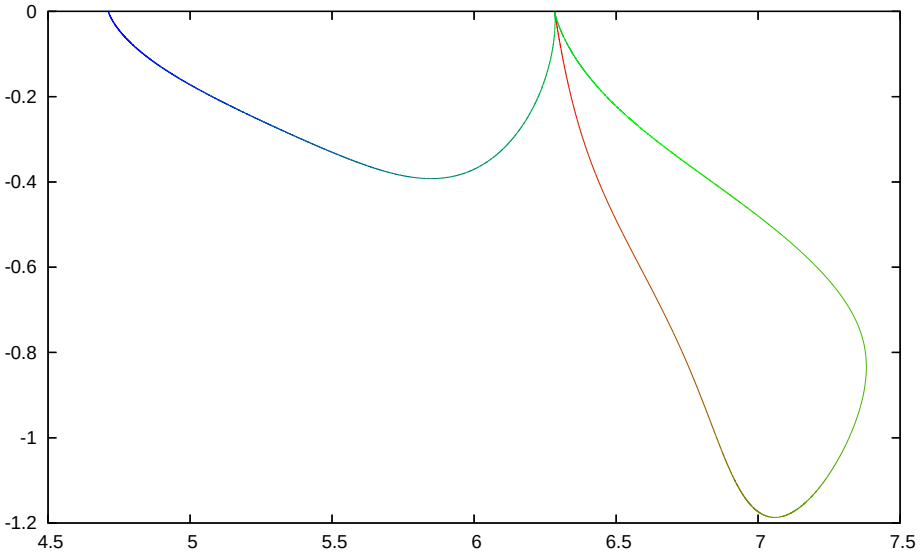

Figure 3.16: The trajectory of the resonance pole $k_0 = 2\pi$ (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha = 3$, $n = 2$. The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

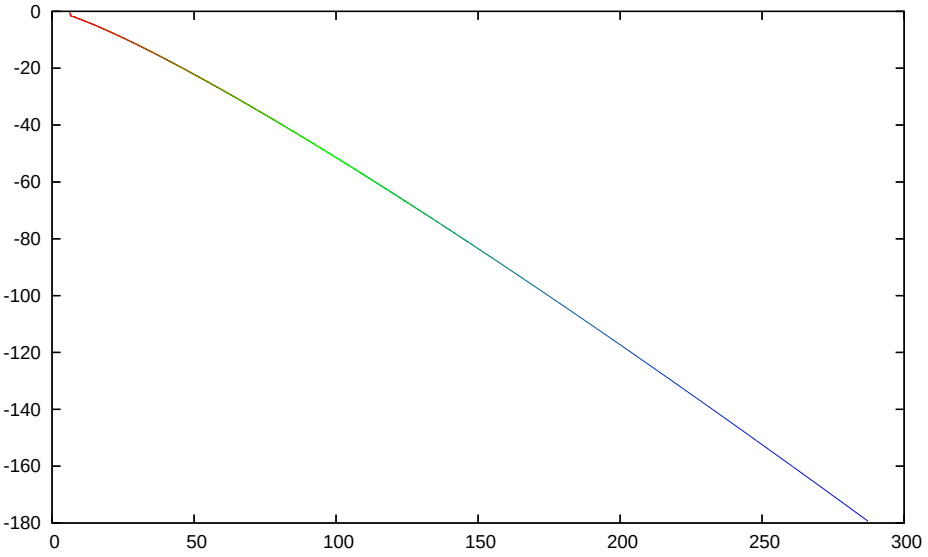

Figure 3.17: The trajectory of the resonance pole $k_0 = 2\pi$ (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha = 1$, $n = 2$. The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

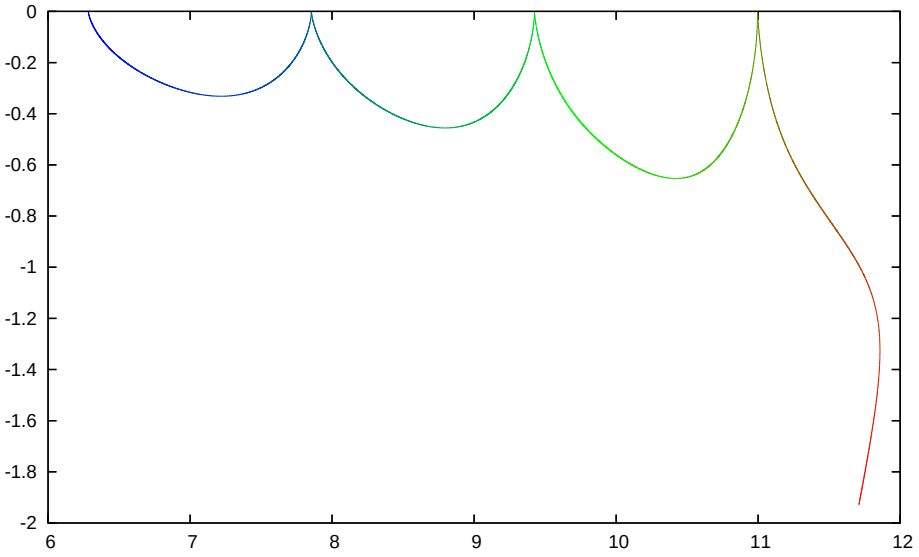

Figure 3.18: The trajectory of the resonance pole (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha = 1$, $n = 2$. The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

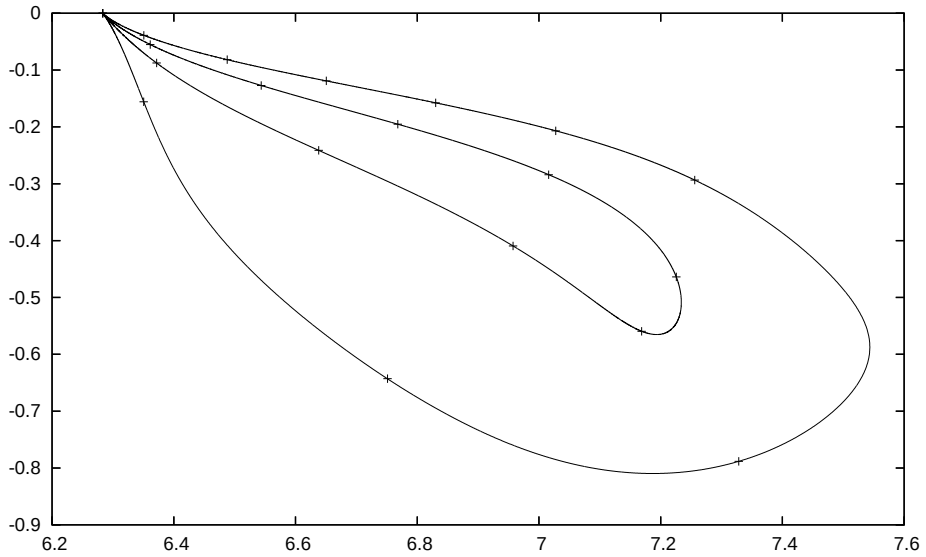

Figure 3.19: A comparison of the trajectory of the resonance pole from the figure 3.15 obtained from the equation (3.7) – the full line – and the resonance poles obtained by numerical solving of the equation (3.6) for λ equal to multiples of 0.05 (represented by crosses). It shows that the error we make by using the approximate equation (3.7) is small (approximately 10^{-4}).

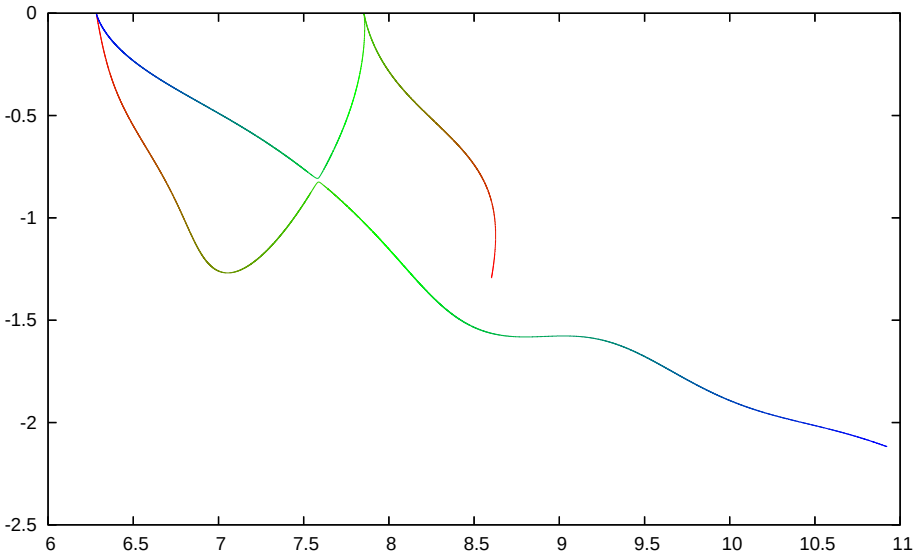

Figure 3.20: The trajectories of two resonance poles (the dependence of the imaginary part of k on the real part of k) for coefficients $\alpha = 2.596$, $n = 2$. We can see the resonance crossing – former eigenvalue embedded into the continuous spectrum changes its place with former resonance (compare, e. g., with figure 3.16). The values of parameter λ are marked by changing the colour of the line from red ($\lambda = 0$) to blue ($\lambda = 1$).

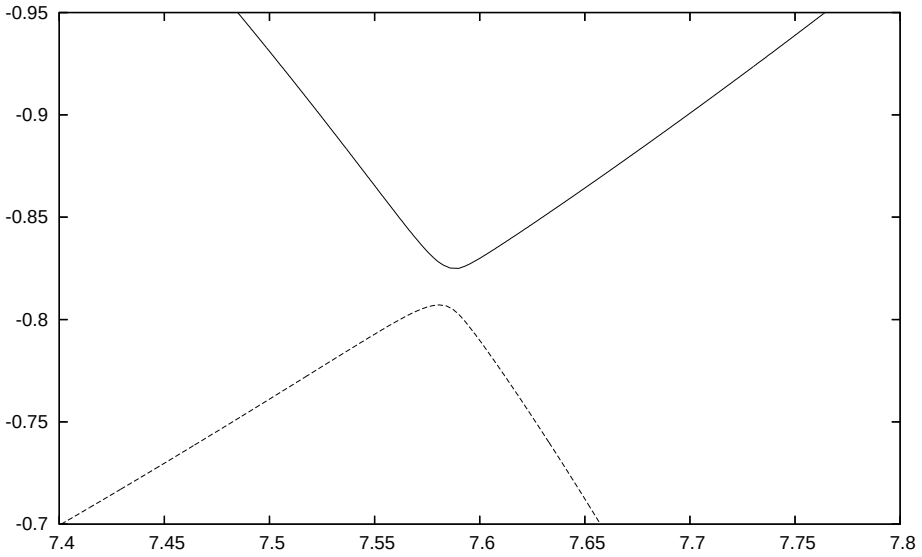

Figure 3.21: A detail of previous figure ($\alpha = 2.596$, $n = 2$).

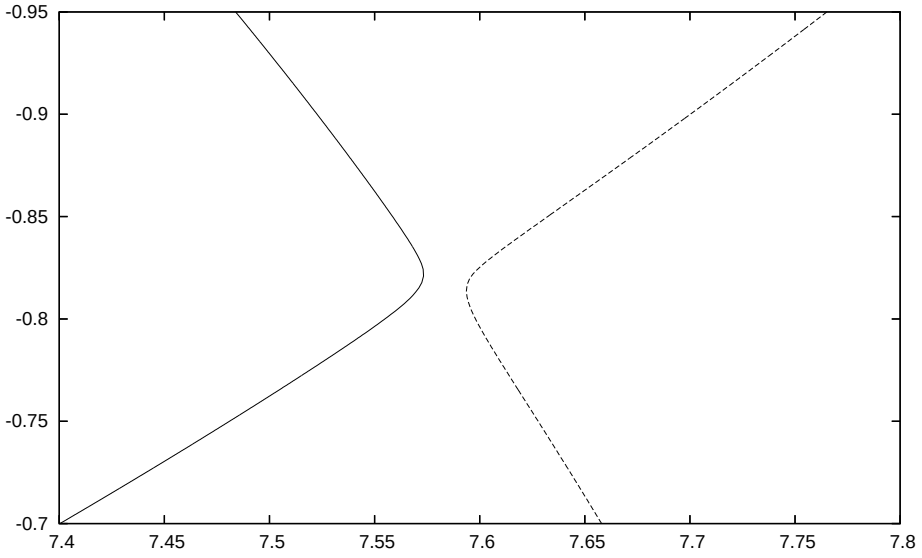

Figure 3.22: A detail similar to figure 3.22, the coefficient α is changed to $\alpha = 2.598$

For example, let us consider the resonator on figure 3.13 again, we change the coupling conditions to Robin conditions at both endpoints and δ-conditions at the middle point (the notation is similar to the example in section 3.2).

$$\begin{aligned} f_1(0) = f_2(0) = g_1(0) = g_2(0)\,, \\ \alpha_1 f_1(l_1) = -f_1'(l_1)\,, \\ \alpha_3 f_1(0) = f_1'(0) + f_2'(0) + g_1'(0) + g_2'(0)\,, \\ \alpha_2 f_2(l_2) = -f_2'(l_2)\,. \end{aligned}$$

We try to find for which coupling constants the poles of the resolvent are real. The lengths of edges l_1, l_2 are given and their rate is not necessarily rational. The condition for poles becomes

$$\begin{vmatrix} -1 & -\cos kl_1 & 0 & 0 & 0 & \sin kl_1 & 0 \\ 0 & \sin kl_1 & 0 & 0 & -1 & \cos kl_1 & 0 \\ 0 & 0 & -1 & -\cos kl_2 & 0 & 0 & \sin kl_2 \\ 0 & 0 & 0 & \sin kl_2 & 0 & -1 & \cos kl_2 \\ k & 0 & 0 & 0 & -\alpha_1 & 0 & 0 \\ 0 & k & k & 0 & 0 & -(\alpha_3 - 2ik) & 0 \\ 0 & 0 & 0 & k & 0 & 0 & -\alpha_2 \end{vmatrix} = 0\,.$$

The imaginary and real part of the determinant give after some arrangements system of equations

$$\begin{aligned} (k\cos kl_1 + \alpha_1 \sin kl_1)(k\cos kl_2 + \alpha_2 \sin kl_2) &= 0\,, \\ (\alpha_1\alpha_2 - k^2)\sin k(l_1+l_2) + k(\alpha_1+\alpha_2)\cos k(l_1+l_3) &= 0\,. \end{aligned}$$

Its solution is

$$\begin{aligned} \alpha_1 &= -k\cot kl_1\,, \\ \alpha_2 &= k\,\frac{\sin k(l_1+l_2) + \cos k(l_1+l_2)\cot kl_1}{\cos k(l_1+l_2) - \sin k(l_1+l_2)\cot kl_1} = -k\cot kl_2\,. \end{aligned}$$

The coefficient α_3 can be chosen arbitrarily which is easy to understand, since the corresponding eigenfunction must be zero at the vertex. Therefore, eigenvalues may be embedded into the continuous spectrum for non-rational rate of the lengths of the edges, too. However, the only way how to get eigenvalues equidistant in the square root for this graph are Neumann or Dirichlet conditions at both end vertices and the rational rate of the lengths of the edges.

3.4 The general case

Let us consider the Hamiltonian acting as $-\mathrm{d}^2/\mathrm{d}x^2$ on a finite quantum graph (i. e., there is no potential on the edges) with the coupling (2.6) – (2.8) and the domain of definition containing functions f with the components $f_{jn} \in W^{2,2}([0, l_{jn}])$.

We express the solutions on the line $\mathcal{L}_{jn}$ as linear combination

$$f_{jn}(x) = a_{jn} \sin kx + b_{jn} \cos kx \,.$$

The identify the point $x = 0$ of the edge with the vertex $\mathcal{X}_j$. From conditions (2.6) – (2.8) we get

$$\begin{aligned} b_j \;&:=\; f_j(j) = b_{jn} \quad \forall n \in \nu(j)\,, \\ f'_{jn}(j) \;&=\; k a_{jn}\,. \end{aligned}$$

We express the transformation between the vector $(a_{jn}, b_j)^T$ and the vector $(a_{nj}, b_n)^T$ corresponding to the other vertex of the edge $\mathcal{X}_n$. From the symmetry of the Ansatz $f_{jn}(x) = f_{nj}(l_{jn} - x)$ we get

$$\begin{aligned} &a_{jn} \sin kx + b_j \cos kx = a_{nj} \sin k(l_{jn} - x) + b_n \cos k(l_{jn} - x) = \\ &= a_{nj}[\sin kl_{jn} \cos kx - \cos kl_{jn} \sin kx] + b_n[\cos kl_{jn} \cos kx + \sin kl_{jn} \sin kx]\,. \end{aligned}$$

Comparing the corresponding terms we obtain

$$\begin{pmatrix} a_{jn} \\ b_j \end{pmatrix} = \begin{pmatrix} -\cos kl_{jn} & \sin kl_{jn} \\ \sin kl_{jn} & \cos kl_{jn} \end{pmatrix} \begin{pmatrix} a_{nj} \\ b_n \end{pmatrix} . \tag{3.9}$$

The set of equations (2.11) becomes

$$\sum_{n \in \nu(j)} a_{jn} = \beta_j(k) k^{-1} b_j \,. \tag{3.10}$$

The system (3.9) and (3.10) represents $\mathrm{card}\mathcal{V} + 2\mathrm{card}\mathcal{L}$ linear equations for the variables a_{jn} and b_j. We denote by $M(k)$ the matrix corresponding to this system, the condition for poles of the resolvent is $\det(M(k)) = 0$.

Let us consider a graph which contains a closed loop of N edges with lengths $l_j = n_j l_0$, $j \in \{1, \dots N\}$, $n_j \in \mathbb{N}$, $l_0 > 0$. Notice, that vertices of the loop may be connected by other lines, see figure 3.23 (the considered loop is plotted with a bold line).

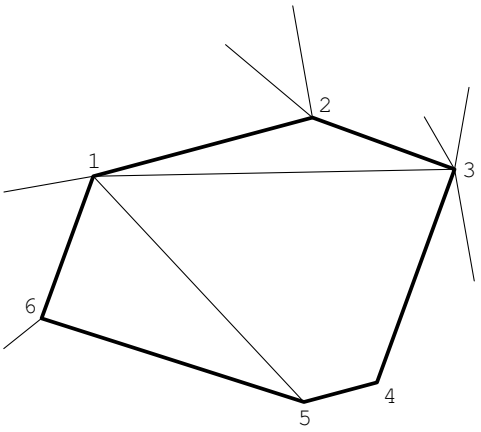

Figure 3.23: An example of a graph containing a loop

Let us express the solutions using coefficients a_{jn} and b_j as before, and the subscripts $i = 1, \dots N$ refer to the vertices of the considered loop. Ordering the variables as $a_{12}, a_{21}, a_{23}, a_{32}, \dots, a_{N1}, a_{1N}, b_1, b_2, \dots, b_N, \dots$ the matrix corresponding to the system of equations (3.9), (3.10) becomes

$$\begin{pmatrix}
-1 & -\cos kl_{12} & 0 & 0\dots & 0 & 0 & 0 & \sin kl_{12} & 0\dots & 0\dots \\
0 & \sin kl_{12} & 0 & 0\dots & 0 & 0 & -1 & \cos kl_{12} & 0\dots & 0\dots \\
0 & 0 & -1 & -\cos kl_{23}\dots & 0 & 0 & 0 & 0 & \sin kl_{23}\dots & 0\dots \\
0 & 0 & 0 & \sin kl_{23}\dots & 0 & 0 & 0 & -1 & \cos kl_{23}\dots & 0\dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0\dots & -1 & -\cos kl_{N1} & \sin kl_{N1} & 0 & 0\dots & 0\dots \\
0 & 0 & 0 & 0\dots & 0 & \sin kl_{N1} & \cos kl_{N1} & 0 & 0\dots & -1\dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & 0 & 0 & 0\dots & 0 & 1 & -\beta_1(k)/k & 0 & 0\dots & 0\dots \\
0 & 1 & 1 & 0\dots & 0 & 0 & 0 & -\beta_2(k)/k & 0\dots & 0\dots \\
0 & 0 & 0 & 0\dots & 1 & 0 & 0 & 0 & 0\dots & -\beta_N(k)/k\dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots
\end{pmatrix}$$

Let us add the columns corresponding to a_{ii+1}, $i = 1, \dots, N$ to the first column and substract the columns corresponding a_{ii-1}. The first column becomes

$$-\left(2\sin^2\frac{kl_{12}}{2}, \sin kl_{12}, \dots, 2\sin^2\frac{kl_{N1}}{2}, \sin kl_{N1}, 0, \dots\right)^T.$$

The terms corresponding to the equations (3.10) disappear and coefficients a_{jn} corresponding to the edges of the loop do not occur in the equations

corresponding to the other edges. Therefore, there are zeros in the first column except of the first $2N$ rows. If the lengths of all the edges in the loop are multiples of l_0 the all the other entries of the first column vanish for $k_0 = 2n\pi/l_0$. Finally, one expands the determinant of the system according to the first column and one can see that the determinant vanishes for $k_0 = 2n\pi/l_0$.

If $\sum_{j=1}^{N} n_j$ is odd then the solutions are $k_0 = 2n\pi/l_0$, $n \in \mathbb{N}$. On the other hand, if the sum is even then we can also find solutions $k_0 = n\pi/l_0$, $n \in \mathbb{N}$.

In the similar way we can proceed if the graph contains a line of edges with rational rate of the lengths and Dirichlet conditions at both ends of the line or Neumann conditions at both ends.

Theorem 3.1. *Let Γ be a quantum graph with coupling conditions (2.6) – (2.8). Let k_0 be a pole of the resolvent of Γ of order n (i.e., solution of $det(M(k)) = 0$). Let us change the lengths of N edges of Γ by $l_i' = l_i(1+\varepsilon_i)$ and denote the changed graph by Γ_ε. Then for sufficiently small $\vec{\varepsilon}$ the resolvent of Γ_ε has either n poles of order 1 or smaller number poles of with the sum of their orders equal to n in the neighbourhood of k_0.*

Proof. We denote by $F(k, \vec{\varepsilon})$ the determinant of the system of equations (3.9), (3.10) for the graph Γ_ε. Because of the form of the equations (3.9), (3.10) and the coefficient $\beta(k)$ it holds that $F(k, \vec{\varepsilon}) \in \mathcal{C}^\infty(\mathbb{C}\backslash\{\mathrm{Im}\, z = 0\} \otimes \mathbb{R}^N)$. If there is the root of the equation $\det(M(k)) = 0$ of order n in k_0 then

$$\left.\frac{\partial^i F(k,\vec{\varepsilon})}{\partial k^i}\right|_{k_0,\vec{\varepsilon}=\vec{0}} = 0 \quad \text{for} \quad i < n\,,$$

$$\left.\frac{\partial^i F(k,\vec{\varepsilon})}{\partial k^i}\right|_{k_0,\vec{\varepsilon}=\vec{0}} \neq 0 \quad \text{for} \quad i = n\,. \tag{3.11}$$

(3.12)

We can use the Taylor expansion

$$\begin{aligned} 0 = F(k,\vec{\varepsilon}) - F(k_0,\vec{0}) &= \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} \frac{1}{p!q!}\frac{\partial^p}{\partial k^p}\frac{\partial^q}{\partial \varepsilon^q} F(k,\varepsilon)\Big|_{k_0,\vec{\varepsilon}=\vec{0}} \\ &= \frac{1}{n!}\left.\frac{\partial^n F(k,\vec{\varepsilon})}{\partial k^n}\right|_{k_0,\vec{\varepsilon}=\vec{0}} \delta k^n + \mathcal{O}(\delta k^{n+1}) + \frac{1}{j!}\left.\frac{\partial^j F(k,\vec{\varepsilon})}{\partial \vec{\varepsilon}^j}\right|_{k_0,\vec{\varepsilon}=\vec{0}} |\vec{\varepsilon}|^j + \\ &\quad + \sum_{p=0}^{n}\sum_{q=0}^{j} \frac{1}{p!q!}\frac{\partial^p}{\partial k^p}\frac{\partial^q}{\partial \varepsilon^q} F(k,\vec{\varepsilon})\Big|_{k_0,\vec{\varepsilon}=\vec{0}} \delta k^p \varepsilon^q + \mathcal{O}(|\vec{\varepsilon}|^{j+1})\,. \end{aligned} \tag{3.13}$$

where $\left.\frac{\partial^j F(k,\vec{\varepsilon})}{\partial \vec{\varepsilon}^j}\right|_{k_0,\vec{\varepsilon}=\vec{0}}$ is the lowest non-zero derivative of F with respect to $\vec{\varepsilon}$ (let us suppose that not all derivatives with respect to $\vec{\varepsilon}$ are equal to zero). We divide the previous equation by the coefficient at the first term (it is nonzero because of 3.11). We denote the two terms with $|\vec{\varepsilon}|^j$ and $\mathcal{O}|\vec{\varepsilon}|^{j+1}$ by a complex number $A_0 \neq 0$; $|A_0|$ is a nonzero number, but it can be chosen arbitrarily small by taking small enough ε. The equation can be rewritten to the form

$$\delta k^n + \sum_{p=1}^{n-1} A_p \delta k^p + A_0 + \mathcal{O}(\delta k^{n+1}) = 0\,, \tag{3.14}$$

where the coefficients A_p could be nonzero but they can be chosen arbitrarily small by taking small enough $|\vec{\varepsilon}|$.

In view of the fundamental theorem of algebra the equation has n solutions. □

Let us summarize our results. If the lengths of all the edges are multiples of l then the spectrum of the graph contains eigenvalues $\epsilon = (2\pi n/l)^2$ (they correspond to $k = 2\pi n/l$). If the sum of lengths of the edges in the loop is an even multiple of l then eigenvalues $\epsilon = (\pi n/l)^2$ (corresponding to $k = \pi n/l$) are present.

Furthermore, we have proved that an eigenvalue of multiplicity n embedded to the continuous spectrum gives raise to n resonances in the spectrum of the perturbed operator or (if the perturbation is chosen appropriately) or a less multiple resonances whereas the sum of multiplicities of all the resonances is equal to n. In other words, the number of poles of the resolvent does not change if their multiplicity is taken into account.

Chapter 4

Star graphs

We will study a star graph with a general coupling at the vertex (schematically illustrated on figure 4.1). It consists of n edges of lengths l_i connected at one endpoint. We assume that there is no potential on the edges, the Hamiltonian act as $-\mathrm{d}^2/\mathrm{d}x^2$. The corresponding Hilbert space is $L^2([0,l_1]) \oplus L^2([0,l_2]) \oplus \cdots \oplus L^2([0,l_n])$, where $x = 0$ corresponds to the connected endpoint. The states are described by the columns $\psi = (f_1, f_2, \dots f_n)^T$.

As it was mentioned in the chapter 2, the coupling in a vertex of a general quantum graph can be described by two square matrices of rank n,

$$A\Psi + B\Psi' = 0\,, \tag{4.1}$$

where Ψ and Ψ' is the vector of the function values at the vertex and the outward derivatives, respectively. For matrices A, B such that (A, B) has

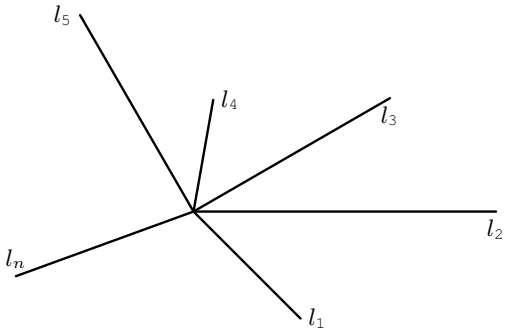

Figure 4.1: An example of a star graph

maximal rank it holds that the Hamiltonian is self-adjoint if and only if the matrix $AB^\dagger$ is self-adjoint at each vertex (see, e. g., [KS99]).

The condition (4.1) can rewritten in the form

$$(U-I)\Psi + iL_0(U+I)\Psi' = 0\,, \tag{4.2}$$

where U is an arbitrary unitary $(n\times n)$ matrix, I is the unit matrix and L_0 is a non-zero constant of length dimension. Having the arguments from the chapter 2 in mind, we can take $L_0 = 1$.

Let us study a star graph with n edges of lengths $l_i > 0$ and the coupling condition (4.2) at the center vertex. For the sake of simplicity, we assume the Dirichlet coupling at the other vertices $f_i(l_i) = 0$. Taking the Ansatz $f_i(x) = a_i \sin k(l_i - x)$ with real constants a_i one gets

$$\Psi = \begin{pmatrix} a_1 \sin kl_1 \\ a_2 \sin kl_2 \\ \vdots \\ a_n \sin kl_n \end{pmatrix} = \begin{pmatrix} \sin kl_1 & 0 & \dots & 0 \\ 0 & \sin kl_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sin kl_n \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix},$$

$$\Psi' = -k \begin{pmatrix} a_1 \cos kl_1 \\ a_2 \cos kl_2 \\ \vdots \\ a_n \cos kl_n \end{pmatrix} = -k \begin{pmatrix} \cos kl_1 & 0 & \dots & 0 \\ 0 & \cos kl_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \cos kl_n \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}.$$

Substituting these expressions (4.2) becomes

$$[(U-I)S(k) - ik(U+I)C(k)](a_1, a_2, \dots, a_n)^T = 0\,,$$

with the matrices $S(k) = \mathrm{diag}\,(\sin kl_1, \sin kl_2, \dots, \sin kl_n)$ and $C(k) = \mathrm{diag}\,(\cos kl_1, \cos kl_2, \dots, \cos kl_n)$. The last equation represents a system of n equations for variables $a_1, a_2, \dots, a_n$. The spectrum of the Hamiltonian is given by the condition of solvability of this system. After some rearrangements we arrive at

$$\det\{U[S(k) - ikC(k)] - [S(k) + ikC(k)]\} = 0\,. \tag{4.3}$$

4.1 Star graph with two edges

Let us begin with a simple example for $n = 2$ (see figure 4.2). The notation is the same as above, the point $x = 0$ corresponds to the center vertex. The Hamiltonian is acting as $-\mathrm{d}^2/\mathrm{d}x^2$, the Hilbert space $L^2([0, l_1]) \oplus L^2([0, l_2])$, i.

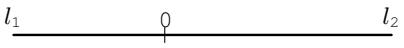

Figure 4.2: A star graph with two edges

e. a state is described by the column $\psi = (f_1, f_2)^T$. The coupling conditions are given by (4.2) and by Dirichlet condition at the other vertices.

Let us derive a suitable parametrization of a U(2) matrix. We denote the components of the matrix U by complex numbers z_{ij}

$$U = \begin{pmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{pmatrix} .$$

Since $UU^\dagger = 1$ the rows of the matrix are orthonormal.

$$\begin{aligned} |z_{11}|^2 + |z_{12}|^2 &= 1\,, \\ |z_{21}|^2 + |z_{22}|^2 &= 1\,, \\ \bar{z}_{11} z_{21} + \bar{z}_{12} z_{22} &= 0 \quad \Rightarrow \quad z_{21} = -\bar{z}_{12} z_{11} z_{22} / |z_{11}|^2\,, \end{aligned}$$

where the overline means complex conjugation. Substituting into the second equation one obtains

$$1 = |z_{22}|^2 (1 + |z_{12}|^2/|z_{11}|^2) = |z_{22}|^2/|z_{11}|^2 \quad \Rightarrow \quad |z_{22}| = |z_{11}|\,.$$

The final parametrization of any element of U(2) group is

$$U = \begin{pmatrix} r\mathrm{e}^{i\varphi_{11}} & \sqrt{1-r^2}\,\mathrm{e}^{i\varphi_{12}} \\ -\sqrt{1-r^2}\,\mathrm{e}^{i(\varphi_{11}+\varphi_{22}-\varphi_{12})} & r\mathrm{e}^{i\varphi_{22}} \end{pmatrix} , \tag{4.4}$$

The condition (4.3) gives $\det M(k) = 0$ where the components of the matrix $M(k)$ are

$$\begin{aligned} m_{11} &= r\mathrm{e}^{i\varphi_{11}}(\sin kl_1 - ik\cos kl_1) - (\sin kl_1 + ik\cos kl_1)\,, \\ m_{12} &= \sqrt{1-r^2}\,\mathrm{e}^{i\varphi_{12}}(\sin kl_2 - ik\cos kl_2)\,, \\ m_{21} &= -\sqrt{1-r^2}\,\mathrm{e}^{i(\varphi_{11}+\varphi_{22}-\varphi_{12})}(\sin kl_1 - ik\cos kl_1)\,, \\ m_{22} &= r\mathrm{e}^{i\varphi_{22}}(\sin kl_2 - ik\cos kl_2) - (\sin kl_2 + ik\cos kl_2)\,. \end{aligned}$$

The condition (4.3) thus can be rewritten as

$$\begin{aligned}
0 = [r\mathrm{e}^{i\varphi_{11}}(\sin kl_1 - ik\cos kl_1) - (\sin kl_1 + ik\cos kl_1)]\cdot \\
\cdot [r\mathrm{e}^{i\varphi_{22}}(\sin kl_2 - ik\cos kl_2) - (\sin kl_2 + ik\cos kl_2)] + \\
+ [\sqrt{1-r^2}\,\mathrm{e}^{i\varphi_{12}}(\sin kl_2 - ik\cos kl_2)]\cdot \\
\cdot [\sqrt{1-r^2}\,\mathrm{e}^{i(\varphi_{11}+\varphi_{22}-\varphi_{12})}(\sin kl_1 - ik\cos kl_1)] = \\
= \mathrm{e}^{i(\varphi_{11}+\varphi_{22})}(\sin kl_1 - ik\cos kl_1)(\sin kl_2 - ik\cos kl_2) - \\
- r\mathrm{e}^{i\varphi_{22}}(\sin kl_1 + ik\cos kl_1)(\sin kl_2 - ik\cos kl_2) - \\
- r\mathrm{e}^{i\varphi_{11}}(\sin kl_1 - ik\cos kl_1)(\sin kl_2 + ik\cos kl_2) + \\
+ (\sin kl_1 - ik\cos kl_1)(\sin kl_2 - ik\cos kl_2)\,.
\end{aligned}$$

Considering different lengths of both edges we generalize the problem discussed in [CFT01b]. While in [CFT01b] the manifold is described by two independent parameters, our manifold is described not only by the eigenvalues of the matrix U but by three parameters $r \in [0,1]$, $\varphi_{11}, \varphi_{22} \in [0, 2\pi)$. To find for which combination of parameters the spectrum does not change we have to compare the coefficients at the linearly independent terms. For $l_1 \neq l_2$ we compare the vectors

$$\begin{pmatrix} \mathrm{e}^{i(\varphi_{11}+\varphi_{22})} \\ r\mathrm{e}^{i\varphi_{11}} \\ r\mathrm{e}^{i\varphi_{22}} \\ 1 \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{i(\varphi'_{11}+\varphi'_{22})} \\ r'\mathrm{e}^{i\varphi'_{11}} \\ r'\mathrm{e}^{i\varphi'_{22}} \\ 1 \end{pmatrix}\,.$$

We obtain

$$\begin{aligned}
& r = r'\,, \\
& r \neq 0 \quad \Rightarrow \quad \varphi_{11} = \varphi'_{11},\ \varphi_{22} = \varphi'_{22}\,, \\
& r = 0 \quad \Rightarrow \quad \varphi_{11} + \varphi_{22} = \varphi'_{11} + \varphi'_{22}\,.
\end{aligned}$$

We can identify the points with $r = 0$ and $\varphi_{11} + \varphi_{22} = \text{const}$. The spectral space is a cube with two pairs of opposite sides identified (because of $\varphi_{11} = 0 \leftrightarrow \varphi_{11} = 2\pi$) and one of the remaining sides shrank into its diagonal.

For $l_1 = l_2 = l$ the vectors

$$\begin{aligned}
(\sin kl_1 + ik\cos kl_1)(\sin kl_2 - ik\cos kl_2) = \sin^2 kl + k^2\cos^2 kl\,, \\
(\sin kl_1 - ik\cos kl_1)(\sin kl_2 + ik\cos kl_2) = \sin^2 kl + k^2\cos^2 kl
\end{aligned}$$

are not linearly independent, hence the proper vectors to compare are

$$\begin{pmatrix} \mathrm{e}^{i(\varphi_{11}+\varphi_{22})} \\ r(\mathrm{e}^{i\varphi_{11}}+\mathrm{e}^{i\varphi_{22}}) \\ 1 \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{i(\varphi'_{11}+\varphi'_{22})} \\ r'(\mathrm{e}^{i\varphi'_{11}}+\mathrm{e}^{i\varphi'_{22}}) \\ 1 \end{pmatrix} .$$

Therefore all the points $(\varphi_{11}, \varphi_{22})$ and $(\varphi_{22}, \varphi_{11})$ could be identified and we obtain in accordance with [CFT01b] the Möbius structure of the spectral space.

4.2 Star graphs with the same length of the edges

As the next step, we investigate graphs with n edges of the same length. The Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$ with the general coupling condition (4.2) again. The corresponding Hilbert space is $L^2([0,l]) \oplus L^2([0,l]) \oplus \cdots \oplus L^2([0,l])$, where $x = 0$ corresponds to the connected endpoint. The states are described by the columns $\psi = (f_1, f_2, \dots f_n)^T$.

Since the matrices in the equation (4.3) are multiples of the unit matrix I

$$S(k) = I \sin kl\,, \quad C(k) = I \cos kl$$

and the determinant of similar matrices is the same the condition (4.3) becomes

$$\begin{aligned} 0 = \det\left[(\sin kl - ik\cos kl)V^{-1}DV - (\sin kl + ik\cos kl)I\right] = \\ = \det\left[(\sin kl - ik\cos kl)D - (\sin kl + ik\cos kl)I\right] \end{aligned}$$

where V is a unitary $n \times n$ matrix and D is a diagonal matrix. It is simple to check that the absolute value of the eigenvalue of an unitary matrix is 1, hence $D = \mathrm{diag}\,(\mathrm{e}^{i\lambda_1}, \mathrm{e}^{i\lambda_2}, \dots, \mathrm{e}^{i\lambda_n})$ with real λ_i.

The condition (4.3) becomes

$$0 = \prod_{j=1}^{n} [\sin kl(\mathrm{e}^{i\lambda_j} - 1) - ik\cos kl(\mathrm{e}^{i\lambda_j} + 1)]\,,$$

i. e.,

$$0 = \prod_{j=1}^{n} \left[\sin kl \sin\frac{\lambda_j}{2} - k\cos kl \cos\frac{\lambda_j}{2}\right] . \tag{4.5}$$

The spectral space is a subset of n-dimensional torus. Any permutation of λ_j does not cause the change of the spectral condition (4.5), hence we can identify these points of the spectral space.

4.3 Star graphs with infinite edges

Let us consider a star graph with no finite edges, but consisting of n halflines connected at one point. We again take the free Hamiltonian acting as $-\mathrm{d}^2/\mathrm{d}x^2$ with coupling conditions (4.2). The corresponding Hilbert space is $L^2([0,\infty)) \oplus L^2([0,\infty)) \oplus \cdots \oplus L^2([0,\infty))$, where $x = 0$ corresponds to the connected endpoint. The states are described by the columns $\psi = (f_1, f_2, \dots f_n)^T$.

The essential spectrum of the Hamiltonian on one halfline with the coupling condition required only at the endpoint is $[0,\infty)$. The coupling conditions at center of the star do not affect the essential spectrum, therefore the essential spectrum of the Hamiltonian on the star graph is $[0,\infty)$ and its multiplicity is given by the number of connected halflines. Since the solution of the Schrödinger equation on the halflines are $\sin kx$ and $\cos kx$ and these functions do not belong to the domain of the Hamiltonian, there are no eigenvalues of this operator.

Let us derive the condition for resonances. Due to the theorem 2.1 we can be satisfied by finding the poles of the S-matrix. Let us take the solutions $f_j(x) = a_j \mathrm{e}^{ikx} + b_j \mathrm{e}^{-ikx}$ on the j-th halfline. Then the condition (4.2) gives

$$(U-I)[(a_1,\dots,a_n)^T+(b_1,\dots,b_n)^T]-k(U+I)[(a_1,\dots,a_n)^T-(b_1,\dots,b_n)^T] = 0\,.$$

Hence

$$[U - I - k(U + I)](a_1,\dots,a_n)^T = -[U - I + k(U + I)](b_1,\dots,b_n)^T\,.$$

The S-matrix maps the vector of the amplitudes of the incoming waves to the vector fo the amplitudes of the outgoing waves ($a = Sb$), therefore its poles are given by the condition

$$0 = \det S^{-1}\,, \quad \Rightarrow \quad 0 = \det\left[U - I - k(U + I)\right].$$

The condition for poles of the S-matrix and consequently also poles of the resolvent is

$$\det\left[(1-k)U - (1+k)I\right] = 0\,.$$

Expressing $U = V^{-1}DV$, $D = \mathrm{diag}\,(\mathrm{e}^{i\lambda_1}, \mathrm{e}^{i\lambda_2}, \dots, \mathrm{e}^{i\lambda_n})$ and using properties of the determinant one obtains

$$0 = \prod_{j=1}^{n}[\mathrm{e}^{i\lambda_j}(1-k) - (1+k)] \quad \Rightarrow \quad 0 = \sin\frac{\lambda_j}{2} + ik\cos\frac{\lambda_j}{2}\,. \tag{4.6}$$

The eigenvalues are $k = i \tan \lambda_j/2$, we choose $\tan \lambda_j/2 > 0$. Since

$$\int_0^\infty \mathrm{e}^{-2 \tan \frac{\lambda_j}{2} x} \, \mathrm{d}x = \frac{1}{2 \tan \frac{\lambda_j}{2}} ,$$

the normalized eigenfunctions corresponding to the eigenvalue $\mathrm{e}^{i\lambda_j}$ are

$$f_i^{(j)}(x) = a_i^{(j)} \sqrt{2 \tan \frac{\lambda_j}{2}} \, \mathrm{e}^{-\tan \frac{\lambda_j}{2} x}$$

with $\sum_{i=1}^n |a_i^{(j)}|^2 = 1$.

4.4 Berry's phase

Let us investigate an interesting property of the model described in the previous section – change of the geometrical phase resulting from the change of the parameter. The total phase gained by a quantum system by the adiabatic evolution consists of a dynamical phase factor and an additional factor. The second factor is called Berry's phase, because of its first description for quantum systems by Berry in [B84].

Let us consider the Hamiltonian with an external time depending parameter $\mathbf{c}(t)$. The eigenstate $|\psi(\mathbf{c}(t))\rangle$ corresponds to the eigenvalue $E(\mathbf{c}(t))$. Let us evolve the eigenvector $|\psi(\mathbf{c}_0)\rangle$ by the Schrödinger equation

$$H(\mathbf{c}(t)) \, |\psi(\mathbf{c}_0), t\rangle = i\hbar \frac{\partial}{\partial t} |\psi(\mathbf{c}_0), t\rangle ,$$

where $\mathbf{c}(0) = \mathbf{c}_0$. The adiabatic theorem states that an eigenvector corresponding to an eigenvalue separated from the rest of the spectrum does not change much under the perturbation small enough. More exactly, with an exponentially small error it follows the "moving eigenstat". For a slow change of the parameter $\mathbf{c}(t)$ the adiabatic theorem can be applied and the eigenvector $|\psi(\mathbf{c}_0), t\rangle$ is therefore proportional to $|\psi(\mathbf{c}(t))\rangle$.

$$|\psi(\mathbf{c}_0), t\rangle \approx \exp\left(-\frac{i}{\hbar} \int_0^t E(\mathbf{c}(t')) \, \mathrm{d}t'\right) \exp\left(i\gamma(t)\right) |\psi(\mathbf{c}(t))\rangle .$$

The first factor means the dynamical phase while γ is the Berry's phase. Substituting into the Schrödinger equation one obtains

$$\frac{\mathrm{d}}{\mathrm{d}t}\gamma(t) = i \langle \psi(\mathbf{c}(t)) | \nabla_{\mathbf{c}} \psi(\mathbf{c}(t)) \rangle \, \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{c}(t) ,$$

which is equivalent to the integral equation

$$\gamma(t) = i \int_{\mathbf{c}_0}^{\mathbf{c}(t)} \langle \psi(\mathbf{c}(t'))|\nabla_{\mathbf{c}}\psi(\mathbf{c}(t'))\rangle \, \mathrm{d}\mathbf{c}(t') \, .$$

For a star graph with infinite edges we investigate a geometrical phase resulting from a change of parameter λ_j for eigenfunction corresponding to the eigenvalue $\mathrm{e}^{i\lambda_j}$ of the matrix U. Then

$$\mathrm{d}f_i^{(j)}(x) = \left(\frac{1}{2\tan\frac{\lambda_j}{2}} - x \right) f_i^{(j)}(x) \frac{\partial \tan\frac{\lambda_j}{2}}{\partial \lambda_j} \, \mathrm{d}\lambda_j \, .$$

Because of

$$\int_0^\infty x \left| f_i^{(j)}(x) \right|^2 \mathrm{d}x = \left| a_i^{(j)} \right|^2 2\tan\frac{\lambda_j}{2} \int_0^\infty x \mathrm{e}^{-2\tan\frac{\lambda_j}{2}x} \, \mathrm{d}x = \frac{\left| a_i^{(j)} \right|^2}{2\tan\frac{\lambda_j}{2}}$$

it holds

$$(f, \mathrm{d}f) = \frac{1}{2\tan\frac{\lambda_j}{2}}(f,f)\frac{\partial \tan\lambda_j/2}{\partial\lambda_j}\mathrm{d}\lambda_j - \frac{1}{2\tan\frac{\lambda_j}{2}}(f,f)\frac{\partial\tan\lambda_j/2}{\partial\lambda_j}\mathrm{d}\lambda_j = 0 \, ,$$

hence the Berry's phase $\int_0^{2\pi} i(f, \mathrm{d}f) \, \mathrm{d}\lambda_j$ is trivial. This is not surprising because the change happens in a one-dimensional subspace.

However, we can get a non-trivial Berry's phase resulting from the change of some parameters of the matrix V. The coefficients of the eigenfunctions for the eigenvalue $\mathrm{e}^{i\lambda_1}$ are given by

$$\begin{pmatrix} a_1^{(1)} \\ a_2^{(1)} \\ \vdots \\ a_n^{(1)} \end{pmatrix} = V^{-1} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \, .$$

Let us study the case $n = 2$, i. e. a quantum graph consisting of two halflines connected at the endpoint with coupling condition (4.2). The matrix V can be parametrized by

$$V = \begin{pmatrix} q & \sqrt{1-q^2}\,\mathrm{e}^{-i\psi} \\ -\sqrt{1-q^2} & q\,\mathrm{e}^{-i\psi} \end{pmatrix} \, , \qquad V^{-1} = \begin{pmatrix} q & -\sqrt{1-q^2} \\ \sqrt{1-q^2}\,\mathrm{e}^{i\psi} & q\,\mathrm{e}^{i\psi} \end{pmatrix} \, .$$

Let us study Berry's phase resulting from the change of parameter ψ. Then

$$f_1^{(1)} = q\mathrm{e}^{-\tan\frac{\lambda_1}{2}x}\sqrt{2\tan\frac{\lambda_1}{2}}\,, \qquad f_2^{(1)} = \sqrt{1-q^2}\mathrm{e}^{i\psi}\mathrm{e}^{-\tan\frac{\lambda_1}{2}x}\sqrt{2\tan\frac{\lambda_1}{2}}\,,$$

and

$$\mathrm{d}f_1^{(1)} = 0\,, \qquad \mathrm{d}f_2^{(1)} = if_2^{(1)}\,\mathrm{d}\psi\,,$$

hence

$$\int_0^{2\pi} i(f,\mathrm{d}f)\,\mathrm{d}\psi = i(-i)\int_0^{2\pi}\int_0^{\infty}(1-q^2)\,\mathrm{e}^{-2\tan\frac{\lambda_1}{2}x}\,2\tan\frac{\lambda_1}{2}\,\mathrm{d}x\,\mathrm{d}\psi = 2\pi(1-q^2)\,.$$

This means that one can obtain any value of Berry's phase $\gamma \in [0, 2\pi)$ by an appropriate choice of parameter q.

Let us compare this result with the one in [EG99]. The coupling parametrization introduced in [EG99] is

$$\Psi' = \begin{pmatrix} a & c \\ \bar{c} & b \end{pmatrix}\Psi\,,$$

comparing with (4.2) one obtains

$$\begin{pmatrix} a & c \\ \bar{c} & b \end{pmatrix} = i(U+I)^{-1}(U-I) = iV^{-1}(D+I)^{-1}(D-I)V\,,$$

where $D = \mathrm{diag}(\mathrm{e}^{i\lambda_1}, \mathrm{e}^{i\lambda_2})$ and therefore

$$(D+I)^{-1}(D-I) = i\,\mathrm{diag}(\tan\lambda_1/2, \tan\lambda_2/2)\,.$$

Now we can continue in comparing both parametrization of the coupling conditions.

$$\begin{pmatrix} a & |c|\,\mathrm{e}^{i\xi} \\ |c|\,\mathrm{e}^{-i\xi} & b \end{pmatrix} = i^2\begin{pmatrix} q & -\sqrt{1-q^2} \\ \sqrt{1-q^2}\,\mathrm{e}^{i\psi} & q\,\mathrm{e}^{i\psi} \end{pmatrix}\cdot$$

$$\cdot\begin{pmatrix} \tan\frac{\lambda_1}{2} & 0 \\ 0 & \tan\frac{\lambda_2}{2} \end{pmatrix}\begin{pmatrix} q & \sqrt{1-q^2}\,\mathrm{e}^{-i\psi} \\ -\sqrt{1-q^2} & q\,\mathrm{e}^{-i\psi} \end{pmatrix} =$$

$$= -\begin{pmatrix} q^2\tan\frac{\lambda_1}{2} + (1-q^2)\tan\frac{\lambda_2}{2} & q\sqrt{1-q^2}\,\mathrm{e}^{-i\psi}(\tan\frac{\lambda_1}{2} - \tan\frac{\lambda_2}{2}) \\ q\sqrt{1-q^2}\,\mathrm{e}^{i\psi}(\tan\frac{\lambda_1}{2} - \tan\frac{\lambda_2}{2}) & (1-q^2)\tan\frac{\lambda_1}{2} + q^2\tan\frac{\lambda_2}{2} \end{pmatrix}\,.$$

Hence

$$\begin{aligned} a &= -\left[q^2 \tan\frac{\lambda_1}{2} + (1-q^2)\tan\frac{\lambda_2}{2}\right], \\ b &= -\left[(1-q^2)\tan\frac{\lambda_1}{2} + q^2\tan\frac{\lambda_2}{2}\right], \\ |c| &= -\left(\tan\frac{\lambda_1}{2} - \tan\frac{\lambda_2}{2}\right) q\sqrt{1-q^2}, \\ \xi &= -\psi. \end{aligned}$$

We can see that the case $a = b$ discussed in [EG99] corresponds to $q^2 = 1/2$ which gives the Berry's phase π.

4.5 High-energy behaviour of the scattering matrix

Let us investigate how the scattering can be affected by the coupling conditions (4.1). The scattering matrix corresponding to the coupling given by matrices A and B can be according to [KS99] expressed as

$$S_{A,B}(k) = -(A + ikB)^{-1}(A - ikB).$$

Denoting $\tilde{B} = -iB$ the last expression could be rewritten as

$$S_{A,B}(k) = \left(\tilde{B} - \frac{1}{k}A\right)^{-1}\left(\tilde{B} + \frac{1}{k}A\right).$$

We are interested in the high-energy asymptotic behaviour. Using the expansion in $1/k$ one gets

$$S_{A,B}(k) = \left(\tilde{B} - \frac{1}{k}A\right)^{-1}\left(\tilde{B} + \frac{1}{k}A\right) = S^{(0)} + \frac{1}{k}S^{(1)} + \frac{1}{k^2}S^{(2)} + \dots .$$

For the sake of simplicity we have omitted the indices corresponding to the matrices A and B for matrices $S^{(i)}$. Now multiplying by $(\tilde{B} - A/k)$ from the left we obtain

$$\tilde{B} + \frac{1}{k}A = \tilde{B}S^{(0)} + \frac{1}{k}\left(\tilde{B}S^{(1)} - AS^{(0)}\right) + \frac{1}{k^2}\left(\tilde{B}S^{(2)} - AS^{(1)}\right) + \dots,$$

i. e., the corresponding set of equation for the matrices $S^{(i)}$ is

$$\tilde{B} = \tilde{B}S^{(0)}, \quad \tilde{B}S^{(1)} = A(S^{(0)} + I), \quad \tilde{B}S^{(i+1)} = AS^{(i)}, \ \forall i \in \mathbb{N}. \qquad (4.7)$$

If the matrix $\tilde{B}$ is invertible then the set of equations (4.7) becomes

$$S^{(0)} = I\,, \quad S^{(1)} = 2\tilde{B}^{-1}A\,, \quad S^{(i+1)} = \tilde{B}^{-1}AS^{(i)}\,,\ \forall i \in \mathbb{N}$$

and the expression of the scattering matrix is

$$\begin{aligned} S_{A,B}(k) &= I + \frac{2}{k}\tilde{B}^{-1}A + \frac{2}{k^2}\tilde{B}^{-1}A\tilde{B}^{-1}A + \cdots = \\ &= I + \frac{2}{k}(U+I)^{-1}(U-I) + \frac{2}{k^2}(U+I)^{-1}(U-I)(U+I)^{-1}(U-I) + \dots\,. \end{aligned} \tag{4.8}$$

However, there are couplings with singular matrix $\tilde{B}$, too. Let us consider the free coupling,

$$\begin{aligned} f_j(0) &= f_k(0)\,, \quad \forall j,k \in \mathbb{N}\,, \\ \sum_j f_j'(0) &= 0\,. \end{aligned}$$

used, e. g., in [BBK00]. The corresponding matrices could be chosen in the following form,

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

From the first two equations in (4.7) we obtain that

$$\sum_{j=1}^{n} S^{(0)}_{ij} = 1\,,\ \forall i\,, \qquad (S^{(0)}+I)_{ij} = (S^{(0)}+I)_{i(j+1)}\,,\ \forall i,j\,.$$

Hence

$$S^{(0)} = \frac{2}{n}\begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \dots & 1 \end{pmatrix} - I\,.$$

From other equations we obtain $S^{(1)} = 0$ and hence $S^{(i)} = 0,\ \forall i \in \mathbb{N}$. Total scattering matrix

$$S_{A,B} = S^{(0)} = \frac{2}{n}\begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \dots & 1 \end{pmatrix} - I\,.$$

is energy independent. Notice, that for these coupling conditions the scattering matrix is equal to unitary matrix U (compare with (2.5)).

The mentioned example corresponds to a more general case.

Proposition 4.1. *The scattering matrix is energy independent if and only if $U^2 = I$. In this case we have $S_U = U$.*

Proof. Let us prove the first implication looking for energy independent scattering matrix. For $S^{(i)} = 0$, $\forall i \in \mathbb{N}$, the condition (4.7) becomes

$$\tilde{B}\left(S^{(0)} - I\right) = 0, \quad A\left(S^{(0)} + I\right) = 0\,.$$

Substituting $A = U - I$, $\tilde{B} = U + I$ the last two equations become

$$\begin{aligned} US^{(0)} + S^{(0)} - U - I &= 0\,, \\ US^{(0)} - S^{(0)} + U - I &= 0 \end{aligned}$$

which is equivalent to

$$US^{(0)} = I\,, \qquad S^{(0)} = U\,.$$

and therefore it gives

$$U^2 = I\,, \qquad S_U = S^{(0)} = U\,.$$

The other implication is also trivial. For $U^2 - I = 0$ the matrices $(U+I)/2$ and $(I-U)/2$ are projectors to the complementary subspaces because of

$$\begin{aligned} \left(\frac{U+I}{2}\right)^2 &= \frac{U^2 + I + 2U}{4} = \frac{U+I}{2}\,, \\ \left(\frac{I-U}{2}\right)^2 &= \frac{U^2 + I - 2U}{4} = \frac{I-U}{2}\,, \\ \frac{U+I}{2} + \frac{I-U}{2} &= I\,. \end{aligned}$$

Hence all the equations in (4.7) except the first one give equalities between two projections to complementary subspaces and therefore

$$(U+I)S^{(i)} = 0\,, \quad (U-I)S^{(i)} = 0 \quad \Rightarrow \quad S^{(i)} = 0\,, \quad \forall i \in \mathbb{N}$$

□

Let us investigate which coupling conditions match to $U^2 = I$ for the simplest nontrivial case $n = 2$. The eigenvalues of the matrix U can be 1 or -1. It is easy to prove that the cases when both of them are equal to 1 and both of them are equal to -1 correspond to Neumann and Dirichlet conditions from both sides of the central vertex, respectively. However, the remaining case with one eigenvalue equal to 1 and the other one equal to -1 provides larger class of coupling conditions. Let us suppose that

$$U = V^{-1} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} V \,,$$

where V is an 2×2 unitary unimodular matrix

$$V = \begin{pmatrix} v_{11} & v_{12} \\ -\bar{v}_{12} & \bar{v}_{11} \end{pmatrix} .$$

The condition (2.2) becomes

$$V^{-1} \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} V \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} + iV^{-1} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} V \begin{pmatrix} \psi_1' \\ \psi_2' \end{pmatrix} = 0 \,.$$

Therefore

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = c_1 \begin{pmatrix} \bar{v}_{11} \\ \bar{v}_{12} \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} ,$$
$$\begin{pmatrix} \psi_1' \\ \psi_2' \end{pmatrix} = c_2 \begin{pmatrix} -v_{12} \\ v_{11} \end{pmatrix} = c \begin{pmatrix} -\bar{z}_2 \\ \bar{z}_1 \end{pmatrix} ,$$

where c_1, c_2 and c are complex constants and $z_1, z_2 \in \mathbb{C}$. The case $z_1 = 0$ corresponds to Dirichlet condition from one side and Neumann from the other one. The case $z_1 = a$, $z_2 = 1$, $c = a^{-1}$ corresponds to

$$\psi_1 = a\psi_2 \,, \quad \psi_1' = -a^{-1}\psi_2' \,.$$

Let us now investigate the remaining case – the matrix $\tilde{B}$ is not invertible but $U^2 \neq I$. Let us rewrite (4.7) using the unitary matrix U.

$$(U + I)(S^{(0)} - I) = 0 \,, \tag{4.9}$$
$$(U - I)(S^{(0)} + I) = (U + I)S^{(1)} \,, \tag{4.10}$$
$$(U - I)S^{(i)} = (U + I)S^{(i+1)} \,, \ \forall i \in \mathbb{N} \,. \tag{4.11}$$

Let U have n_{-1} eigenvalues -1 and n_1 eigenvalues 1. For simplicity, let us study the problem in the basis of eigenvectors of the matrix U. Without

loss of generality we can order the eigenvalues of U in the following way

$$U = \begin{pmatrix} \tilde{U} & 0 & 0 \\ 0 & I_{n_1} & 0 \\ 0 & 0 & -I_{n_{-1}} \end{pmatrix}$$

where $\tilde{U}$ is a diagonal unitary matrix of rank $n - n_{-1} - n_1$ which does not have the eigenvalues 1 and -1, and I_{n_1} and $I_{n_{-1}}$ are unit matrices of rank n_1 or n_{-1}, respectively. For simplicity, we further drop the indices of rank of the unit matrices. We find the properties of the matrices $S^{(i)}$ from the equations (4.9) – (4.11).

From (4.9) we obtain

$$0 = \begin{pmatrix} \tilde{U}+I & 0 & 0 \\ 0 & 2I & 0 \\ 0 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ X & X & X \end{pmatrix} .$$

The elements in the first $n - n_{-1}$ rows of the matrix $S^{(0)} - I$ are equal to zero, because the first $n - n_{-1}$ diagonal elements of the matrix $U + I$ are not trivial. The symbol X means that these blocks of the matrix could contain non-trivial elements.

The rhs of the equation (4.10) has the last n_{-1} rows trivial (for the same reason as before). From the lhs of this equation we obtain

$$\begin{pmatrix} X & X & X \\ X & X & X \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \tilde{U}-I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2I \end{pmatrix} \cdot \begin{pmatrix} X & X & X \\ X & X & X \\ 0 & 0 & 0 \end{pmatrix} .$$

The last n_{-1} rows of the matrix $S^0 + I$ are trivial, hence the matrix $S^{(0)}$ has in the considered basis form

$$S^{(0)} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & -I \end{pmatrix} .$$

The equation (4.10) becomes

$$2 \begin{pmatrix} \tilde{U}-I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \tilde{U}-I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2I \end{pmatrix} \begin{pmatrix} 2I & 0 & 0 \\ 0 & 2I & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \tilde{U}+I & 0 & 0 \\ 0 & 2I & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} M^{(1)} & 0 & 0 \\ 0 & 0 & 0 \\ X & X & X \end{pmatrix}$$

where $M^{(1)} = 2(\tilde{U}+I)^{-1}(\tilde{U}-I)$. If the eigenvalues of the matrix $\tilde{U}$ are $\mathrm{e}^{i\lambda_j}$ then $M^{(1)}$ is a diagonal matrix with elements $2i \tan(\lambda_j/2)$.

From (4.11) we get that the last n_{-1} rows of the matrix $S^{(1)}$ are trivial, hence

$$S^{(1)} = \begin{pmatrix} M^{(1)} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} .$$

Now it is easy to construct from (4.11) the remaining parts of the S-matrix expansion.

$$S^{(i)} = \begin{pmatrix} M^{(i)} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

with $M^{(i)} = 2[(\tilde{U}+I)^{-1}(\tilde{U}-I)]^i$. The scattering matrix can be in the considered basis rewritten in a more compact form

$$S_U(k) = \begin{pmatrix} \tilde{S} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & -I \end{pmatrix} ,$$

where

$$\tilde{S} = I + \sum_{i=1}^{\infty} \frac{1}{k} M^{(i)} = [k(\tilde{U}+I) - (\tilde{U}-I)]^{-1}[k(\tilde{U}+I) + (\tilde{U}-I)] .$$

The matrix $\tilde{S}$ is diagonal and its components are $\frac{k+i\tan\lambda_j/2}{k-i\tan\lambda_j/2} \approx 1+\frac{2i}{k}\tan\lambda_j/2$.

Let us notice that the previous formula holds also for the formerly studied examples. For $U^2 = I$ the eigenvalues are of the matrix U only ± 1 and the matrix $\tilde{S}$ is therefore trivial. If U does not have any eigenvalues -1 we obtain the equation (4.8).

We summarize the obtained results in the following proposition.

Proposition 4.2. *Let U be an unitary matrix of rank n which has n_1 eigenvalues 1 and n_{-1} eigenvalues -1. Let D be a diagonal matrix $D = \mathrm{diag}(\mathrm{e}^{i\lambda_1}, \dots, \mathrm{e}^{i\lambda_{n-n_1-n_{-1}}}, 1, \dots, 1, -1, \dots, -1)$ and $U = V^{-1}DV$. Then the scattering matrix corresponding to the coupling conditions (4.2) for the matrix U is*

$$S_U(k) = V^{-1} \begin{pmatrix} \tilde{S} & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & -I \end{pmatrix} V \approx V^{-1} \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & -I \end{pmatrix} V + \frac{2i}{k} V^{-1} \begin{pmatrix} \tilde{T} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} V ,$$

with

$$\tilde{S} = \mathrm{diag}\left(\frac{k + i\tan(\lambda_1/2)}{k - i\tan(\lambda_1/2)}, \dots, \frac{k + i\tan(\lambda_{n-n_1-n_{-1}}/2)}{k - i\tan(\lambda_{n-n_1-n_{-1}}/2)} \right) .$$

and

$$\tilde{T} = \mathrm{diag}\left(\tan(\lambda_1/2), \ldots, \tan(\lambda_{n-n_1-n_{-1}}/2)\right).$$

This expression of the S-matrix is equivalent to the formula first mentioned by Kostrikin and Schrader

$$S_U(k) = -[U - I - k(U+I)]^{-1}[U - I + k(U+I)], \qquad (4.12)$$

which can be obtained from (4.3).

Let us introduce the explicit form of the scattering matrix for three particular cases mentioned in chapter 2.

For δ-condition it holds $U = \frac{2}{n}J - I$ (see (2.5)), where I is an unitary $n \times n$ matrix and J is a $n \times n$ matrix with all the entries equal to one. After some algebra we arrive using (4.12) at $S_U(k) = \frac{2k}{nk+i\alpha}J - I$, for the simplest cases we have

$$S^{\delta}_{2\times 2}(k) = \begin{pmatrix} \frac{-i\alpha}{2k+i\alpha} & \frac{2k}{2k+i\alpha} \\ \frac{2k}{2k+i\alpha} & \frac{-i\alpha}{2k+i\alpha} \end{pmatrix}, \quad S^{\delta}_{3\times 3}(k) = \begin{pmatrix} \frac{-k-i\alpha}{3k+i\alpha} & \frac{2k}{3k+i\alpha} & \frac{2k}{3k+i\alpha} \\ \frac{2k}{3k+i\alpha} & \frac{-k-i\alpha}{3k+i\alpha} & \frac{2k}{3k+i\alpha} \\ \frac{2k}{3k+i\alpha} & \frac{2k}{3k+i\alpha} & \frac{-k-i\alpha}{3k+i\alpha} \end{pmatrix}.$$

The only case, when the δ-condition give energy independent scattering matrix is $\alpha = 0$, i.e. free coupling condition which were mentioned above.

For δ'_{s}-condition we have $U = I - \frac{2}{n-i\beta}J$, the equation (4.12) gives $S_U(k) = I - \frac{2}{n-ik\beta}J$, for the simplest cases we obtain

$$S^{\delta'_{\mathrm{s}}}_{2\times 2}(k) = \begin{pmatrix} \frac{k\beta}{2i+k\beta} & \frac{-2i}{2i+k\beta} \\ \frac{-2i}{2i+k\beta} & \frac{k\beta}{2i+k\beta} \end{pmatrix}, \quad S^{\delta'_{\mathrm{s}}}_{3\times 3}(k) = \begin{pmatrix} \frac{i+k\beta}{3i+k\beta} & \frac{-2i}{3i+k\beta} & \frac{-2i}{3i+k\beta} \\ \frac{-2i}{3i+k\beta} & \frac{i+k\beta}{3i+k\beta} & \frac{-2i}{3i+k\beta} \\ \frac{-2i}{3i+k\beta} & \frac{-2i}{3i+k\beta} & \frac{i+k\beta}{3i+k\beta} \end{pmatrix}.$$

For δ'-condition we have $U = \frac{2}{n-i\beta}J - \frac{n+i\beta}{n-i\beta}I$, the equation (4.12) gives $S_U(k) = \frac{2}{n-ik\beta}J - \frac{n+ik\beta}{n-ik\beta}I$, for the simplest cases we obtain

$$S^{\delta'}_{2\times 2}(k) = \begin{pmatrix} \frac{k\beta}{2i+k\beta} & \frac{2i}{2i+k\beta} \\ \frac{2i}{2i+k\beta} & \frac{k\beta}{2i+k\beta} \end{pmatrix}, \quad S^{\delta'}_{3\times 3}(k) = \begin{pmatrix} \frac{-i+k\beta}{3i+k\beta} & \frac{2i}{3i+k\beta} & \frac{2i}{3i+k\beta} \\ \frac{2i}{3i+k\beta} & \frac{-i+k\beta}{3i+k\beta} & \frac{2i}{3i+k\beta} \\ \frac{2i}{3i+k\beta} & \frac{2i}{3i+k\beta} & \frac{-i+k\beta}{3i+k\beta} \end{pmatrix}.$$

Notice that the S-matrix can be formally derived from U by replacing α by α/k for δ-condition or by replacing β by $k\beta$ for δ'_{s} and δ'-condition. This is not surprising because the expression of the S-matrix $S = -(A + ikB)^{-1}(A - ikB)$ formally differs from $U = -(A + iB)^{-1}(A - iB)$ only by multiplying the matrix B by k. The connection to the coupling conditions is given by the form of the matrices in chapter 2.

Chapter 5

Tree graphs

5.1 Schrödinger operators on tree graphs

A Schödinger operator on a homogeneous rooted tree graph with free (Kirchhoff) coupling conditions at the vertices is unitarily equivalent to the orthogonal sum of operators acting on $L^2(\mathbb{R}_+)$, as proven by Sobolev and Solomyak in the paper [SS02]. We try to generalize their results to a larger class of coupling conditions and different lengths of the edges. We assume a real bounded and measurable potential $V(|x|)$ on the graph depending only on the distance from the root $|x|$.

Furthermore, we use a similar notation as in [SS02], [EFK07] and [HP06]. Let Γ be a rooted metric tree graph, the root is labeled by o. We denote by $|x|$ the distance between the point x of the graph and the root o. The *branching number* $b(v)$ of the vertex v is the number of vertices emanating from this vertex, i. e., the vertex v connects one edge going from a previous generation with $b(v)$ outgoing edges. In this sense, $b(o) = 1$, for the other vertices we assume $b(v) \geq 1$.

We say that the vertex v of a tree graph Γ belongs to the k-th generation if there are just $k-1$ vertices between v and o ($\operatorname{gen} v = k$). We call the tree graph *regular* if the branching numbers for all the vertices of the same generation are equal and the edges emanating from these vertices have equal length (see figure 5.1). We label the generation of the vertices by $k \geq 0$, so that there are $k-1$ vertices between this vertex and the root. For regular graphs we introduce t_k as the distance between the root and the vertices in the k-th generation and its branching number as b_k. For the root we get $b_0 = 1$ and $t_0 = 0$. Furthermore, one can define the *branching function*

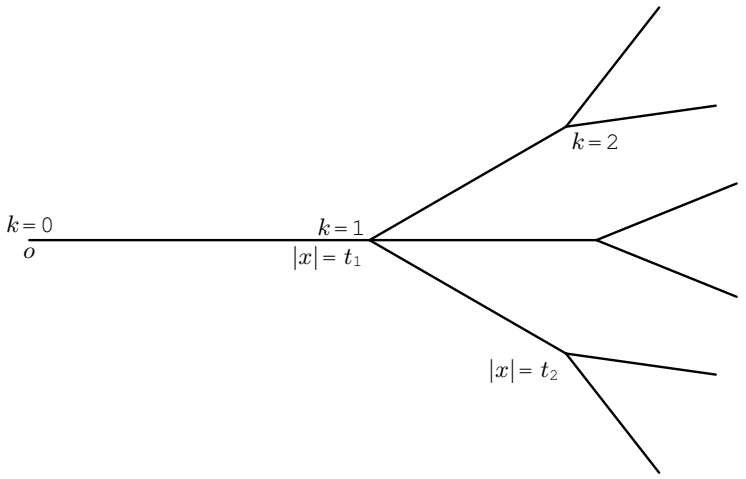

Figure 5.1: An example of a regular tree for $b_0 = 1$, $b_1 = 3$, $b_2 = 2$

$g_0(t) : \mathbb{R}_+ \to \mathbb{N}$ by

$$g_0(t) := b_0 b_1 \dots b_k \quad \text{for} \quad t \in (t_k, t_{k+1}) .$$

The tree graph is called *homogeneous* if there is the same branching number b for all vertices except of o.

One can define order $\succeq$ on set of vertices of the tree graph. We say that vertex w succeeds vertex v ($w \succeq v$) if v lies on the shortest path from o to w. Furthermore, one defines *vertex subtree* $\Gamma_{\succeq v}$ as the set of edges and vertices succeeding v and *edge subtree* $\Gamma_{\succeq e}$ as the union of the edge e and the vertex subtree corresponding to its vertex remoter from the origin.

Let us consider a regular tree graph with the vertex v of the k-th generation and for simplicity denote $b \equiv b_k$. We denote the edges emanating from v by $e_j, j \in \{1, \dots b\}$. Let us consider an operator Q_v on $L^2(\Gamma_{\succeq v})$ which cyclically shifts the functions f_j on edge subtrees $\Gamma_{\succeq e_j}$ in the following way.

$$Q_v : f_j \to f'_j = f_{j+1} ,$$

where we identify f_{b+1} with f_1. Since $Q_v^b = \mathrm{id}$, the operator has eigenvalues $e^s = \mathrm{e}^{is/b}, s \in \{0, \dots, b-1\}$. We denote the corresponding eigenspaces by $L^2_s(\Gamma_{\succeq v}) := \mathrm{Ker}(Q_v - e^s \mathrm{id})$. We call the function $f \in L^2(\Gamma_{\succeq v})$ *s-radial at the vertex* v if and only if $f \in L^2_s(\Gamma_{\succeq v})$ and $f \in L^2_0(\Gamma_{\succeq v'})$ for all vertices v' succeeding v. The set of these functions we denote by $L^2_{s,\mathrm{rad}}(\Gamma_{\succeq v})$. The 0-radial functions are simply called *radial*.

As mentioned in previous chapters, the general coupling at each vertex v is characterized by $(b(v)+1)^2$ parameters or equivalently by an unitary $[(b(v)+1)]\times[(b(v)+1)]$ matrix U_v. In order to get the unitary equivalence with the halfline, we choose only a four-parameter subset, so that all the emanating edges are equivalent. Moreover, the unitary equivalence requires the parameters of the coupling to be equal for all the vertices in same generation. For a vertex v belonging to the k-th generation ($k \geq 1$) the coupling conditions are

$$f_{vj+} = f_{v+}, \qquad \forall j \in \{1,\dots,b(v)\}\,, \tag{5.1}$$

$$\sum_{j=1}^{b(v)} f'_{vj+} - f'_{v-} = \frac{\alpha_{\mathrm{t}k}}{2}(f_{v+}+f_{v-}) + \frac{\gamma_{\mathrm{t}k}}{2}\left(\sum_{j=1}^{b(v)} f'_{vj+} + f'_{v-}\right)\,, \tag{5.2}$$

$$f_{v+} - f_{v-} = -\frac{\bar{\gamma}_{\mathrm{t}k}}{2}(f_{v+}+f_{v-}) + \frac{\beta_{\mathrm{t}k}}{2}\left(\sum_{j=1}^{b(v)} f'_{vj+} + f'_{v-}\right)\,. \tag{5.3}$$

where j distinguishes the edges emanating from v and the subscript minus refers to the ingoing edge. The coefficients $\alpha_{\mathrm{t}k}, \beta_{\mathrm{t}k} \in \mathbb{R}$, $\beta_{\mathrm{t}k} \in \mathbb{C}$ are the same for all the vertices belonging to the k-th generation. The subscript t indicates that they denote the coupling on the tree graph and we will use it in order to avoid confusion in the following chapters. We choose Dirichlet condition at the root,

$$f_o = 0\,. \tag{5.4}$$

Let us denote by $\mathbf{H}$ the Hamiltonian acting as $-\mathrm{d}^2/\mathrm{d}x^2 + V(|x|)$ on a regular tree graph Γ with the branching numbers b_k described above and the potential depending only on the distance from the root. The domain of the Hamiltonian consists of functions $f(x) \in \sum_{e\in\Gamma} \oplus H^2(e)$ satisfying the coupling conditions (5.1) – (5.4). If there is no potential then the Hamiltonian will be denoted by $\mathbf{H}_0$.

In the following text, the Hamiltonian on the tree graph is denoted by a bold $\mathbf{H}$ (or $\mathbf{H}_0$ for a non-potential case) while the corresponding Hamiltonian on the halfline is denoted by H (or H_0).

5.2 Parameterizations of the generalized point interaction

There are multiple ways to describe the four-parameter generalized point interaction (GPI) which connects two leads. Before proceeding with the

construction of the unitary equivalence between Hamiltonian on the graph and direct sum of the Hamiltonians on the halfline, let us summarize the results of [EG99] and [EF06].

First, we compare two different parameterizations connecting two one-dimensional leads proposed in [EG99]. For simplicity, we label the functional value and the derivative from the right by y_+ and y'_+, respectively (similarly for the functional value and derivative from the left). The first of the parameterizations,

$$y'_+ - y'_- = \frac{\alpha}{2}(y_+ + y_-) + \frac{\gamma}{2}(y'_+ + y'_-)\,, \tag{5.5}$$

$$y_+ - y_- = -\frac{\bar\gamma}{2}(y_+ + y_-) + \frac{\beta}{2}(y'_+ + y'_-) \tag{5.6}$$

is characterized by a matrix $\mathcal{A} = \begin{pmatrix} \alpha & \gamma \\ -\bar\gamma & \beta \end{pmatrix}$ with $\alpha, \beta \in \mathbb{R}$ and $\gamma \in \mathbb{C}$. This parameterizations describes almost all selfadjoint extensions of the operator $-\mathrm{d}^2/\mathrm{d}x^2$ restricted to the subspace $\{f \in H^2(\mathbb{R}) : y_+ = y'_+ = y_- = y'_- = 0\}$ except of cases $y_+ = y'_+ = 0$ or $y_- = y'_- = 0$. The form (5.5)–(5.6) can be also easily reduced to the δ-condition case of strength α (requiring $\beta = \gamma = 0$) or the δ'-condition case of strength β (requiring $\alpha = \gamma = 0$).

The second parametrization under consideration is

$$\begin{pmatrix} y'_+ \\ -y'_- \end{pmatrix} = \begin{pmatrix} a & c \\ \bar c & d \end{pmatrix} \begin{pmatrix} y_+ \\ y_- \end{pmatrix}\,, \tag{5.7}$$

with $a, d \in \mathbb{R}$ and $c \in \mathbb{C}$. This parametrization easily decouples the both leads (choosing $c = 0$).

First, we pass from (5.5)–(5.6) to (5.7). We rewrite (5.5) and (5.6) in the form

$$\begin{pmatrix} 1 - \frac{\gamma}{2} & 1 + \frac{\gamma}{2} \\ -\frac{\beta}{2} & \frac{\beta}{2} \end{pmatrix} \begin{pmatrix} y'_+ \\ -y'_- \end{pmatrix} = \begin{pmatrix} \frac{\alpha}{2} & \frac{\alpha}{2} \\ -1 - \frac{\bar\gamma}{2} & 1 - \frac{\bar\gamma}{2} \end{pmatrix} \begin{pmatrix} y_+ \\ y_- \end{pmatrix}\,.$$

Hence

$$\begin{aligned} \begin{pmatrix} a & c \\ \bar c & d \end{pmatrix} &= \begin{pmatrix} 1 - \frac{\gamma}{2} & 1 + \frac{\gamma}{2} \\ -\frac{\beta}{2} & \frac{\beta}{2} \end{pmatrix}^{-1} \begin{pmatrix} \frac{\alpha}{2} & \frac{\alpha}{2} \\ -1 - \frac{\bar\gamma}{2} & 1 - \frac{\bar\gamma}{2} \end{pmatrix} = \\ &= \frac{1}{4\beta} \begin{pmatrix} \alpha\beta + |2+\gamma|^2 & \alpha\beta + (\gamma+2)(\bar\gamma - 2) \\ \alpha\beta + (\gamma-2)(\bar\gamma+2) & \alpha\beta + |2-\gamma|^2 \end{pmatrix} = \\ &= \frac{1}{4\beta} \begin{pmatrix} 4 + \det\mathcal{A} + 4\,\mathrm{Re}\,\gamma & -4 + \det\mathcal{A} - 4i\,\mathrm{Im}\,\gamma \\ -4 + \det\mathcal{A} + 4i\,\mathrm{Im}\,\gamma & 4 + \det\mathcal{A} - 4\,\mathrm{Re}\,\gamma \end{pmatrix}\,. \end{aligned}$$

Notice that the parametrization (5.7) does not contain the case $\beta = 0$, i.a., the δ-interaction.

For the passage from (5.7) to (5.5)–(5.6) it is convenient to introduce another basis

$$\begin{aligned} g_1 &= y_+ + y_- \,, \quad g_2 = y'_+ + y'_- \,, \\ g_3 &= y_+ - y_- \,, \quad g_4 = y'_+ - y'_- \,. \end{aligned}$$

Using the reverse relations

$$\begin{aligned} y_+ &= \frac{g_1 + g_3}{2} \,, \quad y_- = \frac{g_1 - g_3}{2} \,, \\ y'_+ &= \frac{g_2 + g_4}{2} \,, - \quad y'_- = \frac{g_4 - g_2}{2} \end{aligned}$$

one can rewrite the equation (5.7) as

$$\begin{pmatrix} 1 & c-a \\ 1 & d-\bar{c} \end{pmatrix} \begin{pmatrix} g_4 \\ g_3 \end{pmatrix} = \begin{pmatrix} a+c & -1 \\ d+\bar{c} & 1 \end{pmatrix} \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}$$

and therefore

$$\begin{aligned} \begin{pmatrix} \alpha & \gamma \\ -\bar{\gamma} & \beta \end{pmatrix} &= 2 \cdot \begin{pmatrix} 1 & c-a \\ 1 & d-\bar{c} \end{pmatrix}^{-1} \begin{pmatrix} a+c & -1 \\ d+\bar{c} & 1 \end{pmatrix} = \\ &= \frac{4}{a+d-2\operatorname{Re} c} \begin{pmatrix} ad-|c|^2 & \frac{1}{2}(a-d) - i \operatorname{Im} c \\ -\frac{1}{2}(a-d) - i \operatorname{Im} c & 1 \end{pmatrix} . \end{aligned}$$

Lemma 5.1. *The correspondence of the coupling conditions (5.5) – (5.6) and (5.7) is given by*

$$\begin{aligned} \begin{pmatrix} a & c \\ \bar{c} & d \end{pmatrix} &= \frac{1}{4\beta} \begin{pmatrix} 4 + \det\mathcal{A} + 4\operatorname{Re}\gamma & -4 + \det\mathcal{A} - 4i\operatorname{Im}\gamma \\ -4 + \det\mathcal{A} + 4i\operatorname{Im}\gamma & 4 + \det\mathcal{A} - 4\operatorname{Re}\gamma \end{pmatrix} , \\ \begin{pmatrix} \alpha & \gamma \\ -\bar{\gamma} & \beta \end{pmatrix} &= \frac{4}{a+d-2\operatorname{Re} c} \begin{pmatrix} ad-|c|^2 & \frac{1}{2}(a-d) - i \operatorname{Im} c \\ -\frac{1}{2}(a-d) - i \operatorname{Im} c & 1 \end{pmatrix} . \end{aligned}$$

Another possibility of parametrization is using the 2x2 unitary matrix U mentioned in the previous chapters.

$$(U - I) \begin{pmatrix} y_+ \\ y_- \end{pmatrix} + i(U + I) \begin{pmatrix} y'_+ \\ -y'_- \end{pmatrix} = 0$$

where

$$U = \mathrm{e}^{i\xi} \begin{pmatrix} u_1 & u_2 \\ -\bar{u}_2 & \bar{u}_1 \end{pmatrix} .$$

with $u_1, u_2 \in \mathbb{C}$, $|u_1|^2 + |u_2|^2 = 1$ and $\xi \in [0, \pi)$. The relation to the parametrization (5.5) – (5.6) is according to [EF06]

$$\begin{aligned} u_1 &= \frac{-2(\alpha+\beta) + 4i\,\mathrm{Re}\,\gamma}{\sqrt{(\alpha\beta+|\gamma|^2)^2 + 4\alpha^2 + 4\beta^2 + 8|\gamma|^2 + 16}}\,, \\ u_2 &= \frac{1}{2i}\frac{\alpha\beta + |\gamma|^2 - 4 - 4i\,\mathrm{Im}\,\gamma}{\sqrt{(\alpha\beta+|\gamma|^2)^2 + 4\alpha^2 + 4\beta^2 + 8|\gamma|^2 + 16}}\,, \\ \tan\xi &= \frac{\alpha\beta + |\gamma|^2 + 4}{2(\alpha-\beta)}\,. \end{aligned}$$

5.3 Mapping of the coupling conditions to the halfline

In this section, we find out which coupling conditions on the halfline correspond to (5.1) – (5.4). First, let us outline the main idea of the unitary equivalence between the graph and the halfline — identification of a "symetric" function $f \in L^2_{0,\mathrm{rad}}(\Gamma)$ with the function on a halfline. One constructs the isometry $\Pi : f \to \varphi$, $\varphi(t) = f(x)$ for $t = |x|$ of $L^2_{0,\mathrm{rad}}(\Gamma)$ into the weighted space $L^2(\mathbb{R}_+, g_0)$ with the norm

$$\|\varphi\|^2_{L^2(\mathbb{R}_+,g_0)} = \int_{\mathbb{R}_+} |\varphi(t)|^2 g_0(t)\,\mathrm{d}t\,.$$

Furthermore, one passes to $L^2(\mathbb{R})$ by $y(t) = g_0^{1/2}(t)\varphi(t)$ using the map defined by

$$\|y\|^2_{L^2(\mathbb{R}_+)} = \|\varphi\|^2_{L^2(\mathbb{R}_+,g_0)}$$

which is an isometry, and the relations

$$\begin{aligned} y_{k+} &= (b_0 \cdot \ldots \cdot b_k)^{1/2}\varphi_{k+}\,, \\ y_{k-} &= (b_0 \cdot \ldots \cdot b_{k-1})^{1/2}\varphi_{k-}\,, \end{aligned}$$

at the vertices.

We can substitute these relations into (5.1) – (5.4) and divide both sides of these four equations by $(b_0 \ldots b_{k-1})^{-1/2}$. Due to the linearity of the coupling conditions (5.1) – (5.4) the passage from $f(x)$ to $y(t)$ is for the vertex from the k-th generation equivalent to the change

$$f_{v-} \to y_{k-}\ , \quad f'_{v-} \to y'_{k-}\,, \tag{5.8}$$

$$f_{v+} \to b_k^{-1/2} y_{k+}\ , \quad \sum_{j=1}^{b_k} f_{v+} \to b_k^{1/2} y_{k+}\,. \tag{5.9}$$

Since the rearranging of the equations (5.1) – (5.4) after substitutions (5.8) – (5.9) into the form (5.5) – (5.6) is technically more difficult, we first investigate the change of the coupling

$$\begin{pmatrix} \sum_{j=1}^{b} f'_{j+} \\ -f'_{-} \end{pmatrix} = \begin{pmatrix} a_{\rm t} & c_{\rm t} \\ \bar{c}_{\rm t} & d_{\rm t} \end{pmatrix} \begin{pmatrix} f_{+} \\ f_{-} \end{pmatrix} , \tag{5.10}$$

which corresponds to the parametrization (5.7). For simplicity, we have omitted the indices v and k. Using (5.8) – (5.9) one obtains

$$\begin{pmatrix} y'_{+} \\ -y'_{-} \end{pmatrix} = \begin{pmatrix} b^{-1}a_{\rm t} & b^{-1/2}\, c_{\rm t} \\ b^{-1/2}\, \bar{c}_{\rm t} & d_{\rm t} \end{pmatrix} \begin{pmatrix} y_{+} \\ y_{-} \end{pmatrix} ,$$

therefore the coupling parameters for the halfline are

$$a_{\rm h} = b^{-1}a_{\rm t} , \quad c_{\rm h} = b^{-1/2}c_{\rm t} , \quad d_{\rm h} = d_{\rm t} .$$

If $\beta_{\rm t} \neq 0$ we can use the relations from lemma (5.1) to show the correspondence of the parameters of the coupling (5.1) – (5.4) and the coupling (5.5) – (5.6) on the halfline.

$$\alpha_{\rm h} = \frac{4b^{-1}(a_{\rm t}\, d_{\rm t} - |c_{\rm t}|^2)}{b^{-1}a_{\rm t} + d_{\rm t} - 2b^{-1/2}\,{\rm Re}\, c_{\rm t}} = \\ = \frac{16\alpha_{\rm t}}{4(b^{1/2}+1)^2 + {\rm det}\mathcal{A}_{\rm t}(b^{1/2}-1)^2 + 4(1-b)\,{\rm Re}\,\gamma_{\rm t}} ,$$

$$\beta_{\rm h} = \frac{4}{b^{-1}a_{\rm t} + d_{\rm t} - 2b^{-1/2}\,{\rm Re}\, c_{\rm t}} = \\ = \frac{16\, b\, \beta_{\rm t}}{4(b^{1/2}+1)^2 + {\rm det}\mathcal{A}_{\rm t}(b^{1/2}-1)^2 + 4(1-b)\,{\rm Re}\,\gamma_{\rm t}} ,$$

$$\gamma_{\rm h} = \frac{2(b^{-1}a_{\rm t} - d_{\rm t} - 2ib^{-1/2}\,{\rm Im}\, c_{\rm t})}{b^{-1}a_{\rm t} + d_{\rm t} - 2b^{-1/2}\,{\rm Re}\, c_{\rm t}} = \\ = 2 \cdot \frac{(1-b)(4+{\rm det}\mathcal{A}_{\rm t}) + 8ib^{1/2}\,{\rm Im}\,\gamma_{\rm t} + 4(b+1)\,{\rm Re}\,\gamma_{\rm t}}{4(b^{1/2}+1)^2 + {\rm det}\mathcal{A}_{\rm t}(b^{1/2}-1)^2 + 4(1-b)\,{\rm Re}\,\gamma_{\rm t}} .$$

To solve the case $\beta_{\rm t} = 0$ one can use the basis g_i, $i = 1, \ldots, 4$ introduced in previous section. The transformation (5.8) – (5.9) becomes

$$g_1 \to \frac{b^{-1/2}+1}{2}\tilde{g}_1 + \frac{b^{-1/2}-1}{2}\tilde{g}_3 , \quad g_2 \to \frac{b^{1/2}+1}{2}\tilde{g}_2 + \frac{b^{1/2}-1}{2}\tilde{g}_4 ,$$
$$g_3 \to \frac{b^{-1/2}+1}{2}\tilde{g}_3 + \frac{b^{-1/2}-1}{2}\tilde{g}_1 , \quad g_4 \to \frac{b^{1/2}+1}{2}\tilde{g}_4 + \frac{b^{1/2}-1}{2}\tilde{g}_2 .$$

The coupling conditions

$$\begin{pmatrix} g_4 \\ g_3 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \alpha_{\rm t} & \gamma_{\rm t} \\ \bar{\gamma}_{\rm t} & \beta_{\rm t} \end{pmatrix} \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}$$

become

$$\frac{b^{1/2}-1}{2}\tilde{g}_2 + \frac{b^{1/2+1}}{2}\tilde{g}_4 = \\ = \frac{1}{2}\left(\alpha_{\rm t}\frac{b^{-1/2}+1}{2}\tilde{g}_1 + \alpha_{\rm t}\frac{b^{-1/2}-1}{2}\tilde{g}_3 + \gamma_{\rm t}\frac{b^{1/2}+1}{2}\tilde{g}_2 + \gamma_{\rm t}\frac{b^{1/2}-1}{2}\tilde{g}_4 \right),$$

$$\frac{b^{-1/2}-1}{2}\tilde{g}_1 + \frac{b^{-1/2}+1}{2}\tilde{g}_3 = \frac{1}{2}\left(-\bar{\gamma}_{\rm t}\frac{b^{-1/2}+1}{2}\tilde{g}_1 - \bar{\gamma}_{\rm t}\frac{b^{-1/2}-1}{2}\tilde{g}_3 \right).$$

From the second equation one obtains

$$\gamma_{\rm h} = 2 \cdot \frac{2(b^{-1/2}-1)+\gamma_{\rm t}(b^{-1/2}+1)}{2(b^{-1/2}+1)+\gamma_{\rm t}(b^{-1/2}-1)} = \\ = 2 \cdot \frac{(1-b)(4+|\gamma_{\rm t}|^2) + 8ib^{1/2}\,{\rm Im}\,\gamma_{\rm t} + 4(b+1)\,{\rm Re}\,\gamma_{\rm t}}{4(b^{1/2}+1)^2 + |\gamma_{\rm t}|^2(b^{1/2}-1)^2 + 4(1-b)\,{\rm Re}\,\gamma_{\rm t}}.$$

Subsequently

$$\alpha_{\rm h} = \frac{\frac{b^{-1/2}+1}{2} - \frac{\gamma_{\rm h}}{2}\frac{b^{-1/2}-1}{2}}{\frac{b^{1/2}+1}{2} - \frac{\gamma_{\rm t}}{2}\frac{b^{1/2}-1}{2}} = \\ = \frac{16\alpha_{\rm t}}{4(b^{1/2}+1)^2 + |\gamma_{\rm t}|^2(b^{1/2}-1)^2 + 4(1-b)\,{\rm Re}\,\gamma_{\rm t}}$$

and trivially $\beta_{\rm h} = 0$.

Therefore, the form of the term computed for $\beta_{\rm t} \neq 0$ can be used also for $\beta_{\rm t} = 0$.

The case when the denominators of the terms are zero corresponds to $y_+ = -y_-$, $y'_+ = -y'_-$. The Hamiltonian with mentioned conditions is unitarily equivalent to the free Hamiltonian.

Obviously, the Dirichlet or Neumann conditions do not change under the transformation (5.8) – (5.9).

$$f_+ = f_- = 0 \quad \Rightarrow \quad y_+ = y_- = 0\,, \\ \sum_{j=1}^{b} f'_{j+} = f'_- = 0 \quad \Rightarrow \quad y'_+ = y'_- = 0\,,$$

Let us summarize the results of this section.

Lemma 5.2. *The coupling conditions (5.1) – (5.4) change under the transformation (5.8) – (5.9) to*

$$\begin{aligned} y'_{k+} - y'_{k-} &= \frac{\alpha_{\mathrm{h}}}{2}(y_{k+} + y_{k-}) + \frac{\gamma_{\mathrm{h}}}{2}(y'_{k+} - y'_{k-})\,, \\ y_{k+} - y_{k-} &= -\frac{\bar{\gamma}_{\mathrm{h}}}{2}(y_{k+} + y_{k-}) + \frac{\beta_{\mathrm{h}}}{2}(y'_{k+} - y'_{k-})\,, \\ y(0+) &= 0\,, \end{aligned}$$

where

$$\begin{aligned} \alpha_{\mathrm{h}} &= \frac{16\alpha_{\mathrm{t}}}{4(b^{1/2}+1)^2 + \det\mathcal{A}_{\mathrm{t}}(b^{1/2}-1)^2 + 4(1-b)\operatorname{Re}\gamma_{\mathrm{t}}}\,, \\ \beta_{\mathrm{h}} &= \frac{16\,b\,\beta_{\mathrm{t}}}{4(b^{1/2}+1)^2 + \det\mathcal{A}_{\mathrm{t}}(b^{1/2}-1)^2 + 4(1-b)\operatorname{Re}\gamma_{\mathrm{t}}}\,, \\ \gamma_{\mathrm{h}} &= 2\,\cdot\,\frac{(1-b)(4+\det\mathcal{A}_{\mathrm{t}}) + 8ib^{1/2}\operatorname{Im}\gamma_{\mathrm{t}} + 4(b+1)\operatorname{Re}\gamma_{\mathrm{t}}}{4(b^{1/2}+1)^2 + \det\mathcal{A}_{\mathrm{t}}(b^{1/2}-1)^2 + 4(1-b)\operatorname{Re}\gamma_{\mathrm{t}}}\,. \end{aligned}$$

The conditions $f_{v+} = f_{v-} = 0$ *or* $\sum_{j=1}^{b_k} f'_{vj+} = f'_{v-} = 0$ *transform to* $y_{k+} = y_{k-} = 0$ *or* $y'_{k+} = y'_{k-} = 0$*, respectively.*

5.4 Construction of the unitary equivalence

In this section we show the decomposition of $L_2(\Gamma)$ into subspaces of the radial functions and, subsequently, the equivalence of Hamiltonian on a tree graph to the orthogonal sum of Hamiltonians on the halfline. We proceed similarly to appendix A in [HP06].

Let us define a quantum graph L_n as a halfline parametrized by $t \in (t_n, \infty)$ with coupling conditions from lemma 5.2 at points $t_k, k > n$ and Dirichlet condition at t_n. Let us define the operator J_{vs} acting from $L^2_{s,\mathrm{rad}}(\Gamma_{\succeq v})$ to the halfline $L^2(L_n)$ by

$$J_{vs} f := \bigoplus_{k>n} (b_n \cdot \dots \cdot b_{k-1})^{1/2}\ f|_{\Gamma_k}\ .$$

Lemma 5.3. *The operator* J_{vs} *is unitary.*

Proof.

$$\|J_{vs}\|^2_{L_n} = \sum_{k>n} (b_n \cdot \dots \cdot b_{k-1})\,\|f\|^2_{\Gamma_k} = \|f\|^2_{\Gamma_{\succeq v}}$$

□

Lemma 5.4. *We can decompose*

$$L^2(\Gamma) = L^2_{0,\mathrm{rad}}(\Gamma) \bigoplus_{\substack{v\in\Gamma\\ v\neq o}} \bigoplus_{s=1}^{b(v)-1} L^2_{s,\mathrm{rad}}(\Gamma_{\succeq v})\,.$$

Proof. For every vertex v belonging to the k-th generation one can use the eigenspace decomposition of the operator Q_v defined in section 5.1

$$L^2(\Gamma_{\succeq v}) = \bigoplus_{s=0}^{b_k-1} L^2_s(\Gamma_{\succeq v})\,. \tag{5.11}$$

Furthermore, we have decomposition

$$L^2_s(\Gamma_{\succeq v}) = L^2_{s,\mathrm{rad}}(\Gamma_{\succeq v}) \bigoplus_{\substack{w\in\Gamma, w\succeq v\\ \mathrm{gen}\, w=\mathrm{gen}\, v+1}} \left(L^2_s(\Gamma_{\succeq w}) \ominus L^2_{s,\mathrm{rad}}(\Gamma_{\succeq w})\right)\,. \tag{5.12}$$

From (5.11) we have

$$L^2(\Gamma_{\succeq v}) \ominus L^2_{0,\mathrm{rad}}(\Gamma_{\succeq v}) = \bigoplus_{s=1}^{b_k-1} L^2_s(\Gamma_{\succeq v})\,,$$

because of $L^2_0(\Gamma_{\succeq v}) = L^2_{0,\mathrm{rad}}(\Gamma_{\succeq v})$. Substituting it into (5.12) one obtains

$$\begin{aligned} L^2(\Gamma) = L^2_{0,\mathrm{rad}}(\Gamma_{\succeq o}) \bigoplus_{s=1}^{b_1-1} L^2_s(\Gamma_{\succeq o_1}) = \\ = L^2_{0,\mathrm{rad}}(\Gamma_{\succeq o}) \bigoplus_{s=1}^{b_1-1} L^2_{s,\mathrm{rad}}(\Gamma_{\succeq o_1}) \bigoplus_{\substack{v\in\Gamma\\ \mathrm{gen}\, v=2}} \bigoplus_{s=1}^{b_2-1} L^2_s(\Gamma_{\succeq v})\,, \end{aligned}$$

where o_1 is the only vertex belonging to the first generation. Repeating this substitution, one obtains the desired decomposition. □

Our aim is now to extend this decomposition to the domain of the Hamiltonian.

Let us define for a given vertex v and $s = 1, \ldots, b(v) - 1$

$$\begin{aligned} \mathrm{dom}\, \mathbf{H}_{vs,\mathrm{rad}} = \{f \in \bigoplus_{e\in\Gamma_{\succeq v}} H^2(\Gamma_{\succeq v})\,|\, f \in L^2_{s,\,\mathrm{rad}}(\Gamma_{\succeq v}), f_{v+} = 0, \\ f \text{ satisfies (5.1) – (5.3) for all } w \succeq v\}\,. \end{aligned}$$

Now we show the decomposition for domains of the mentioned Hamiltonians.

Lemma 5.5. *One can decompose*

$$\operatorname{dom}\mathbf{H} = \operatorname{dom}\mathbf{H}_{o0,\mathrm{rad}} \bigoplus_{\substack{v\in\Gamma\\ v\neq o}} \bigoplus_{s=1}^{b(v)-1} \operatorname{dom}\mathbf{H}_{vs,\mathrm{rad}}\,.$$

Proof. By definition, $\operatorname{dom}\mathbf{H}_{o0,\mathrm{rad}} \subset L^2_{o0,\mathrm{rad}}(\Gamma_{\succeq v})$ and $\operatorname{dom}\mathbf{H}_{vs,\mathrm{rad}} \subset L^2_{vs,\mathrm{rad}}(\Gamma)$ for all $s = 1,\dots,b(v)$. Furthermore, we realize that a function from $\operatorname{dom}\mathbf{H}_{vs,\mathrm{rad}}$ satisfies $\sum_{j=1}^{b(v)} f'_{vj+} = 0$. Therefore, it does not influence the fulfilment of the coupling conditions (5.1) – (5.3) and the orthogonal sum belongs to $\operatorname{dom}\mathbf{H}$. In other words, the function from $\operatorname{dom}\mathbf{H}$ can be decomposed to the function from $\operatorname{dom}\mathbf{H}_{o0,\mathrm{rad}}$ and functions $\operatorname{dom}\mathbf{H}_{o_1 s,\mathrm{rad}}$, where o_1 is the vertex of the first generation. The first one guaranties the fulfilment of the coupling conditions at o_1, addition of the other functions does not change the coupling conditions. □

Lemma 5.6. *Let v be a vertex belonging to the n-th generation. The Hamiltonian $\mathbf{H}_{vs,\mathrm{rad}}$ is unitary equivalent to the Hamiltonian $\mathbf{H}_{L_n}$ where $n = \mathrm{gen}v$*

$$\mathbf{H}_{L_n}(y) := -\frac{\mathrm{d}^2}{\mathrm{d}t^2} + V(t)$$

With the domain consisting of functions in $f \in \bigoplus_{k=n}^{\infty} H^2(t_k, t_{k+1})$ satisfying the conditions from lemma 5.2 in $t_k, k > n$ and $y = 0$ for t_n.

Proof. The proof follows from lemmas 5.2 and 5.3. □

We can summarize the results in following theorem.

Theorem 5.1. *The Hamiltonian $\mathbf{H}$ on a radial tree graph Γ is unitary equivalent to*

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

where $(\oplus m)H_{L_n}$ is the m-multiple copy of the operator H_{L_n}.

Similarly to [HP06], our results can be generalized also to so-called tree-like graphs (the edges emanating from the vertices of the same generation are replaced by the same compact graph).

5.5 Spectrum of the operator $\mathbf{H}_0$

In this section, we construct the spectrum of the operator $\mathbf{H}_0$ with concrete coupling conditions. We denote by $\mathbf{H}_0(\mathcal{A}_\mathrm{t}, l)$ the operator $\mathbf{H}_0$ with the length l of all the edges and coupling conditions (5.2) – (5.3) given by the same matrix $\mathcal{A}_\mathrm{t}$ at all the vertices except of the root and Dirichlet condition at the root. We denote by $H_0(\mathcal{A}_\mathrm{h}, l)$ the corresponding operator on the halfline and we find its spectrum.

Let us first explore the case $c_\mathrm{h} = 0$ where all the parts of the halfline are separated. The spectrum is purely point and is obtained by solving the problem of infinitely many abscissae with the same coupling conditions (5.7) and the first one with Dirichlet condition at one end. The coupling conditions (5.7) become

$$y'_+ = a_\mathrm{h} y_+ \,, \quad -y'_- = d_\mathrm{h} y_- \,.$$

Using Ansatz $y_n(s) = A_n \sin ks + B_n \cos ks$, $t = s + t_n$ for $t \in (t_n, t_{n+1})$, $n > 0$ we arrive at

$$\begin{aligned} y_n(0+) &= B_n \,, & y_n(l-) &= A_n \sin kl + B_n \cos kl \,, \\ y'_n(0+) &= kA_n \,, & y'_n(l-) &= kA_n \cos kl - kB_n \sin kl \,. \end{aligned}$$

The equation

$$\begin{pmatrix} k & -a_\mathrm{h} \\ d_\mathrm{h} \sin kl + k \cos kl & d_\mathrm{h} \cos kl - k \sin kl \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix} = 0$$

is solvable for

$$(a_\mathrm{h} d_\mathrm{h} - k^2) \sin kl + k(a_\mathrm{h} + d_\mathrm{h}) \cos kl = 0 \,. \tag{5.13}$$

Similarly, the problem on the first abscissa gives the condition

$$0 = \det \begin{pmatrix} 0 & -1 \\ d_\mathrm{h} \sin kl + k \cos kl & d_\mathrm{h} \cos kl - k \sin kl \end{pmatrix} = d_\mathrm{h} \sin kl + k \cos kl \,. \tag{5.14}$$

The following theorem summarizes this case for the parametrization (5.5) – (5.6).

Theorem 5.2. *The operator $H_0(\mathcal{A}_\mathrm{h}, l)$ has for the separating conditions $\det \mathcal{A}_\mathrm{h} = 4$ and $\operatorname{Im} \gamma = 0$ only the point spectrum. It consists of the points $\epsilon = k^2$ given by the equation*

$$(\alpha_\mathrm{h} - k^2 \beta_\mathrm{h}) \sin kl + 4k \cos kl = 0$$

of infinite multiplicity and the points given by the equation

$$(2 - \operatorname{Re}\gamma_{\mathrm{h}}) \sin kl + \beta_{\mathrm{h}} k \cos kl = 0$$

of the multiplicity one.

Proof. The spectrum is given by the equations (5.13) – (5.14) above. One can use the lemma (5.1) to obtain the spectral conditions in the parametrization (5.5) – (5.6). □

In the following, we suppose that $c_{\mathrm{h}} \neq 0$.

To obtain the essential spectrum of the operator $H_0(\mathcal{A}_{\mathrm{h}}, l)$, let us define the operator $H'(\mathcal{A}_{\mathrm{h}}, l)$ as the Laplacian on $\mathbb{R}$ with the domain consisting of functions in $\oplus_{j=-\infty}^{\infty} H^2(jl, (j+1)l)$ and the coupling conditions (5.5) – (5.6) given by the matrix $\mathcal{A}_{\mathrm{h}}$ for each point $j \in \mathbb{Z}$.

Lemma 5.7. *The essential spectrum of the operator $H_0(\mathcal{A}_{\mathrm{h}}, l)$ coincides with the essential spectrum of the operator $H'(\mathcal{A}_{\mathrm{h}}, l)$.*

Proof. The proof is similar to the proof of theorem 3.2 in [SS02]. Let us consider the operator $H_0(\mathcal{A}_{\mathrm{h}}, l)$ with the Dirichlet condition in $t = 0$ and conditions (5.5) – (5.6) in $n \in \mathbb{N}$. One can obtain the essential spectrum of this operator by the similar procedure as in [SS02]. One defines the operator D on $L^2(\mathbb{R}_+)$ by

$$(Dy)(t) = -iy'(t)$$

and coupling conditions (5.5) – (5.6) in $n \in \mathbb{N}$. Using its adjoint $D^\dagger$, one can express the operator $H_0(\mathcal{A}_{\mathrm{h}}, l) = D^\dagger D$ and denote by $H_0'(\mathcal{A}_{\mathrm{h}}, l)$ the operator on $L^2(\mathbb{R}_-)$ which can be obtained from $DD^\dagger$ using substitution $t \to -t$.

Then the operator $H''(\mathcal{A}_{\mathrm{h}}, l) = H_0'(\mathcal{A}_{\mathrm{h}}, l) \oplus H_0(\mathcal{A}_{\mathrm{h}}, l)$ has matching conditions $y(0+) = 0$, $y'(0-) = 0$ and (5.5) – (5.6) for $n \in \mathbb{Z}\backslash\{0\}$. Hence the essential spectrum of the operator $H'(\mathcal{A}_{\mathrm{h}}, l)$ coincides with the essential spectrum of the operator $H''(\mathcal{A}_{\mathrm{h}}, l)$, i. e., the union of essential spectra of the operators $H_0'(\mathcal{A}_{\mathrm{h}}, l)$ and $H_0(\mathcal{A}_{\mathrm{h}}, l)$. Therefore, the essential spectrum is given by bands in the theorem 4.1 in [EG99] of multiplicity two. □

5.5.1 The essential spectrum of the operator $H'(\mathcal{A}_{\mathrm{h}}, l)$

The band spectrum of this operator is given by the theorem 4.1 in [EG99]. We proceed using Bloch decomposition and reduce the problem on $(-l/2, l/2)$ with coupling conditions

$$y(-l/2) = \mathrm{e}^{i\theta} y(l/2)\,, \quad y'(-l/2) = \mathrm{e}^{i\theta} y'(l/2) \tag{5.15}$$

and the conditions (5.5) – (5.6) at $t = 0$.

Using Ansatz $y(t) = A_1 \mathrm{e}^{ikt/2} + A_2 \mathrm{e}^{-ikt/2}$, $t \in (-l/2, 0)$ and $y(t) = A_3 \mathrm{e}^{ikt/2} + A_4 \mathrm{e}^{-ikt/2}$, $t \in (0, l/2)$ one obtains from (5.15) and (5.5) – (5.6) four equations for variables $A_1, \ldots, A_4$.

$$
\begin{aligned}
ik(-A_1 + A_2 + A_3 - A_4) &= \\
&= \frac{\alpha_\mathrm{h}}{2}(A_1 + A_2 + A_3 + A_4) + ik\frac{\gamma_\mathrm{h}}{2}(A_1 - A_2 + A_3 - A_4)\,, \\
-A_1 - A_2 + A_3 + A_4 &= \\
&= -\frac{\bar\gamma_\mathrm{h}}{2}(A_1 + A_2 + A_3 + A_4) + ik\frac{\beta_\mathrm{h}}{2}(A_1 - A_2 + A_3 - A_4)\,, \\
A_1 \mathrm{e}^{-ikl/2} + A_2 \mathrm{e}^{ikl/2} &= A_3 \mathrm{e}^{i\theta + ikl/2} + A_4 \mathrm{e}^{i\theta - ikl/2}\,, \\
ik(A_1 \mathrm{e}^{-ikl/2} - A_2 \mathrm{e}^{ikl/2}) &= ik(A_3 \mathrm{e}^{i\theta + ikl/2} - A_4 \mathrm{e}^{i\theta - ikl/2})\,.
\end{aligned}
$$

The determinant of this system of equations is

$$
\begin{vmatrix}
\frac{\alpha_\mathrm{h}}{2} + ik(1 + \frac{\gamma_\mathrm{h}}{2}) & \frac{\alpha_\mathrm{h}}{2} - ik(1 + \frac{\gamma_\mathrm{h}}{2}) & \frac{\alpha_\mathrm{h}}{2} - ik(1 - \frac{\gamma_\mathrm{h}}{2}) & \frac{\alpha_\mathrm{h}}{2} + ik(1 - \frac{\gamma_\mathrm{h}}{2}) \\
1 - \frac{\bar\gamma_\mathrm{h}}{2} + ik\frac{\beta_\mathrm{h}}{2} & 1 - \frac{\bar\gamma_\mathrm{h}}{2} - ik\frac{\beta_\mathrm{h}}{2} & -1 - \frac{\bar\gamma_\mathrm{h}}{2} + ik\frac{\beta_\mathrm{h}}{2} & -1 - \frac{\bar\gamma_\mathrm{h}}{2} - ik\frac{\beta_\mathrm{h}}{2} \\
\mathrm{e}^{-ikl/2} & \mathrm{e}^{ikl/2} & -\mathrm{e}^{i(\theta + kl/2)} & -\mathrm{e}^{i(\theta - kl/2)} \\
\mathrm{e}^{-ikl/2} & -\mathrm{e}^{ikl/2} & -\mathrm{e}^{i(\theta + kl/2)} & \mathrm{e}^{i(\theta - kl/2)}
\end{vmatrix}\,.
$$

Requiring the determinant to be zero, one obtains

$$
\begin{aligned}
\mathrm{e}^{2i\theta}(-4ik + 2ik\bar\gamma_\mathrm{h} + ik\alpha_\mathrm{h}\beta_\mathrm{h} - 2ik\gamma_\mathrm{h} + ik|\gamma_\mathrm{h}|^2) + \mathrm{e}^{i\theta}(4ik\mathrm{e}^{-ikl} + \\
+ 4ik\mathrm{e}^{ikl} - 2\alpha_\mathrm{h}\mathrm{e}^{-ikl} + 2\alpha_\mathrm{h}\mathrm{e}^{ikl} + 2k^2\beta_\mathrm{h}\mathrm{e}^{-ikl} - 2k^2\beta_\mathrm{h}\mathrm{e}^{-ikl}) - \\
- 4ik - 2ik\bar\gamma_\mathrm{h} + ik\alpha_\mathrm{h}\beta_\mathrm{h} + 2ik\gamma_\mathrm{h} + ik|\gamma_\mathrm{h}|^2 = 0\,,
\end{aligned}
$$

which yields

$$
\mathrm{Re}\,[(4 - \det \mathcal{A}_\mathrm{h} + 4i\,\mathrm{Im}\,\gamma_\mathrm{h})\,\mathrm{e}^{i\theta}] = (4 + \det \mathcal{A}_\mathrm{h})\cos kl + \frac{2}{k}(\alpha_\mathrm{h} - \beta_\mathrm{h}k^2)\sin kl\,. \tag{5.16}
$$

The essential spectrum consists of bands Δ_m. In the following theorem we examine four different cases of high-energy behaviour.

Theorem 5.3. *The essential spectrum of the operator $H'(\mathcal{A}_\mathrm{h}, l)$ is consists for non-separating $\mathcal{A}_\mathrm{h}$ ($\det \mathcal{A}_\mathrm{h} \neq 4$ or $\mathrm{Im}\,\gamma_\mathrm{h} \neq 0$) of spectral bands Δ_m.*

a) If $\beta_\mathrm{h} \neq 0$ then the bands are centered approximately near

$$
\epsilon_m = (k + \delta k)^2 = \frac{\pi^2 m^2}{l^2} + \frac{(4 + \det \mathcal{A}_\mathrm{h})}{\beta_\mathrm{h} l} + \mathcal{O}(m^{-1})\,.
$$

and their width is

$$|\Delta_m(\mathcal{A}_{\rm h}, l)| = 2k\delta k = \frac{\sqrt{(4+\det \mathcal{A}_{\rm h})^2 + 16\,(\mathrm{Im}\,\gamma_{\rm h})^2}}{|\beta_{\rm h}|l}\,.$$

b) If $\beta_{\rm h} = 0$ *and* $\mathrm{Re}\,\gamma_{\rm h} \neq 0$ *then the bands are centered approximately near*

$$\epsilon_m = (k+\delta k)^2 = \frac{(2m+1)^2\pi^2}{4l^2} + \frac{4\alpha_{\rm h}}{(4+|\gamma_{\rm h}|^2)l} + \mathcal{O}(m^{-1})\,.$$

and their width is

$$|\Delta_m(\mathcal{A}_{\rm h}, l)| = 2k\delta k = \frac{4\pi m}{l}\arcsin\frac{\sqrt{(4-|\gamma_{\rm h}|^2)^2 + 16|\mathrm{Im}\,\gamma_{\rm h}|^2}}{4+|\gamma_{\rm h}|^2}\,.$$

c) If $\beta_{\rm h} = 0$ *and* $\mathrm{Re}\,\gamma_{\rm h} = 0$ *then the width of the gaps is*

$$|\Gamma_m(\mathcal{A}_{\rm h}, l)| = \frac{8\alpha_{\rm h}}{(4+|\gamma_{\rm h}|^2)l} + \mathcal{O}(m^{-1})\,.$$

Proof. a) If $\beta_{\rm h} \neq 0$ then the rhs of the equation (5.16) is dominated by the term $-2k\beta_{\rm h}\sin kl$. We expand the rhs around zeros of the dominative term $k = m\pi/l$, $m \in \mathbb{Z}$.

$$k = \frac{m\pi}{l} + \delta k \quad \Rightarrow \quad \cos kl \approx (-1)^m\,, \quad \sin kl \approx (-1)^m\delta k\,.$$

Putting the lhs to be zero and using the high-energy limit one obtains

$$0 \approx (4+\det\mathcal{A}_{\rm h})(-1)^m - 2\beta_{\rm h}\frac{\pi m}{l}(-1)^m\delta k \quad \Rightarrow \quad \delta kl = \frac{(4+\det\mathcal{A}_{\rm h})}{2\pi m\beta_{\rm h}}\,.$$

Therefore, the approximate center of the bands is

$$\epsilon_m = (k+\delta k)^2 = \frac{\pi^2 m^2}{l^2} + \frac{(4+\det\mathcal{A}_{\rm h})}{\beta_{\rm h} l} + \mathcal{O}(m^{-1})\,.$$

The absolute value of the number on the lhs is $\sqrt{(4+\det\mathcal{A}_{\rm h})^2 + 16\,(\mathrm{Im}\,\gamma_{\rm h})^2}$. The widths of the bands can be determined from the relation

$$2\sqrt{(4+\det\mathcal{A}_{\rm h})^2 + 16(\,\mathrm{Im}\,\gamma_{\rm h})^2} \approx \left|\left.\frac{\mathrm{d}\,\mathrm{rhs}}{\mathrm{d}k}\right|_{k=\frac{\pi m}{l}}\delta k\right| \approx |-2\beta_{\rm h} l(-1)^m lk\delta k\,,$$

therefore,

$$|\Delta_m(\mathcal{A}_{\rm h}, l)| = 2k\delta k = \frac{\sqrt{(4+\det\mathcal{A}_{\rm h})^2 + 16\,(\mathrm{Im}\,\gamma_{\rm h})^2}}{|\beta_{\rm h}|l}\,.$$

b) If $\beta_{\rm h} = 0$ and $\mathrm{Re}\,\gamma_{\rm h}$ then the condition 5.16 simplifies to

$$\mathrm{Re}\left(\frac{4 - |\gamma_{\rm h}|^2 + 4i\,\mathrm{Im}\,\gamma_{\rm h}}{4 + |\gamma_{\rm h}|^2}\right) = \cos kl + \frac{2\alpha_{\rm h}}{k(4 + |\gamma_{\rm h}|^2)} \sin kl\,.$$

The rhs is dominated by the first term, we expand the rhs around $k = (2m+1)\pi/(2l)$, $m \in \mathbb{Z}$.

$$k = \frac{(2m+1)\pi}{2l} + \delta k \quad \Rightarrow \quad \cos kl \approx -(-1)^m l\delta k\,, \quad \sin kl \approx (-1)^m\,.$$

Using the high-energy limit one obtains

$$0 \approx -(-1)^m \delta k\, l + (-1)^m \frac{4l\alpha_{\rm h}}{\pi(2m+1)(4 + |\gamma_{\rm h}|^2)}\,,$$

$$\delta k \approx \frac{4\alpha_{\rm h}}{\pi(2m+1)(4 + |\gamma_{\rm h}|^2)}\,.$$

The approximate center of the bands is

$$\epsilon_m = (k + \delta k)^2 = \frac{(2m+1)^2\pi^2}{4l^2} + \frac{4\alpha_{\rm h}}{(4 + |\gamma_{\rm h}|^2)l} + \mathcal{O}(m^{-1})\,.$$

The widths of the bands can be determined from the relation

$$\delta k \approx \frac{2}{l} \arcsin \frac{\sqrt{(4 - |\gamma_{\rm h}|^2)^2 + 16|\mathrm{Im}\,\gamma_{\rm h}|^2}}{4 + |\gamma_{\rm h}|^2}\,,$$

therefore,

$$|\Delta_m(\mathcal{A}_{\rm h}, l)| = 2k\delta k = \frac{4\pi m}{l} \arcsin \frac{\sqrt{(4 - |\gamma_{\rm h}|^2)^2 + 16|\mathrm{Im}\,\gamma_{\rm h}|^2}}{4 + |\gamma_{\rm h}|^2}\,.$$

c) The case $\beta = 0$, $\mathrm{Re}\,\gamma = 0$ follows from theorem 2.2.3 on page 271 of [AB] with α replaced by $\alpha_{\rm h}/(4 + |\gamma_{\rm h}|^2)$.

□

5.5.2 The point spectrum of the operator $H_0(\mathcal{A}_{\rm h}, l)$

Let us construct the eigenfunctions of the operator $H_0(\mathcal{A}_{\rm h}, l)$. For simplicity, we drop the index h. We choose the Ansatz

$$y(t) = A_j \sin ks + B_j \cos ks, \quad \text{for } t \in ((j-1)l, jl),\ s = t - (j-1)l\,.$$

Hence

$$\begin{aligned} y(jl+) &= B_j\,, \qquad y(jl-) = A_{j-1}\sin kl + B_{j-1}\cos kl\,,\\ y'(jl+) &= kA_j\,, \qquad y'(jl-) = k(A_{j-1}\cos kl - B_{j-1}\sin kl)\,. \end{aligned}$$

Using the parametrization (5.7) one obtains

$$\begin{aligned} kA_{j+1} &= aB_{j+1} + cA_j\sin kl + cB_j\cos kl\,,\\ kB_j\sin kl - kA_j\cos kl &= \bar{c}B_{j+1} + dA_j\sin kl + dB_j\cos kl\,, \end{aligned}$$

which can be rewritten to the form

$$\begin{pmatrix} k & -a\\ 0 & -\bar{c}\end{pmatrix}\begin{pmatrix} A_{j+1}\\ B_{j+1}\end{pmatrix} = \begin{pmatrix} c\sin kl & c\cos kl\\ d\sin kl + k\cos kl & d\cos kl - k\sin kl\end{pmatrix}\begin{pmatrix} A_j\\ B_j\end{pmatrix}\,.$$

For $c=0$ and $k=0$ there is an inversion of the matrix on the lhs.

$$\begin{pmatrix} A_{j+1}\\ B_{j+1}\end{pmatrix} = \frac{1}{\bar{c}k}\begin{pmatrix} \bar{c} & -a\\ 0 & -k\end{pmatrix}\begin{pmatrix} c\sin kl & c\cos kl\\ d\sin kl + k\cos kl & d\cos kl - k\sin kl\end{pmatrix}\begin{pmatrix} A_j\\ B_j\end{pmatrix} =$$
$$= \frac{1}{\bar{c}k}\begin{pmatrix} (|c|^2 - ad)\sin kl - ak\cos kl & (|c|^2 - ad)\cos kl + ak\sin kl\\ -dk\sin kl - k^2\cos kl & -dk\cos kl + k^2\sin kl\end{pmatrix}\begin{pmatrix} A_j\\ B_j\end{pmatrix}\,.$$

Denoting the last matrix by $M(k,\mathcal{A})$ we have

$$\begin{pmatrix} A_{j+1}\\ B_{j+1}\end{pmatrix} = M(k,\mathcal{A})\begin{pmatrix} A_j\\ B_j\end{pmatrix}\,. \tag{5.17}$$

The norm of the function $y(t)$ is

$$\begin{aligned} \|y\|^2 &= \sum_{j=1}^{\infty}\int_0^l |A_j\sin ks + B_j\cos ks|^2\,\mathrm{d}s =\\ &= \sum_{j=1}^{\infty}\int_0^l [|A_j|^2\sin^2 ks + |B_j|^2\sin^2 ks + 2\,\mathrm{Re}\,(A_j\bar{B}_j)\sin ks\cos ks]\,\mathrm{d}s\,. \end{aligned}$$

We can restrict ourselves to the real or pure imaginary k only, since the operator $H_0(\mathcal{A}_{\mathrm{h}},l)$ is selfadjoint. Using

$$\begin{aligned} \int_0^l \sin^2 kl\,\mathrm{d}x &= \frac{1}{4k}[(2kl)^2 - \sin 2kl]\,,\\ \int_0^l \cos^2 kl\,\mathrm{d}x &= \frac{1}{4k}[(2kl)^2 + \sin 2kl]\,,\\ \int_0^l \sin kl\cos kl\,\mathrm{d}x &= -\frac{1}{4k}\cos 2kl \end{aligned}$$

one obtains

$$\|y\|^2 = \sum_{j=1}^{\infty} \frac{1}{4k}[|A_j|^2((2kl)^2 - \sin 2kl) + |B_j|^2((2kl)^2 + \sin 2kl) + \\ + 2\,\mathrm{Re}\,(A_j\bar{B}_j)(-\cos 2kl)]\,. \quad (5.18)$$

Notice that $M(k,\mathcal{A})$ depends only on k and the coefficients of the matrix $\mathcal{A}$. Therefore, for given energy we have

$$A_{j+1} = (1,0)M^j(k,\mathcal{A})\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}\,, \quad B_{j+1} = (0,1)M^j(k,\mathcal{A})\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}\,.$$

Dirichlet condition at $t = 0$ corresponds to $B_1 = 0$, $A_1 = A$. Furthermore, let $M = U^\dagger DU$, where D is diagonal and U unitary matrix.

Let λ_+ and λ_- be eigenvalues of the matrix M and $D = \mathrm{diag}\,(\lambda_+, \lambda_-)$. Then

$$A_j = A(1,0)U^\dagger \begin{pmatrix} |\lambda_+|^j & 0 \\ 0 & |\lambda_-|^j \end{pmatrix} U \begin{pmatrix} 1 \\ 0 \end{pmatrix}\,.$$

Similarly, for B_j one obtains

$$B_j = A(0,1)U^\dagger \begin{pmatrix} |\lambda_+|^j & 0 \\ 0 & |\lambda_-|^j \end{pmatrix} U \begin{pmatrix} 1 \\ 0 \end{pmatrix}\,.$$

For other coupling conditions at the root we can use the projection to another vector.

The eigenvalues of the matrix $M(k,\mathcal{A})$ are

$$\lambda_\pm = \frac{1}{2\bar{c}k}\left\{-(a+d)k\cos kl + (k^2 + |c|^2 - ad)\sin kl \pm \right. \\ \left. \pm \sqrt{[-(a+d)k\cos kl + (k^2+|c|^2-ad)\sin kl]^2 - 4|c|^2k^2}\right\}\,,$$

which can be rewritten in the form

$$\lambda_\pm = \mathrm{e}^{i\varphi}\left(\lambda_0 \pm \sqrt{\lambda_0^2 - 1}\right)\,,$$

where

$$\lambda_0 = \frac{1}{2|c|k}\left[-(a+d)k\cos kl + (k^2+|c|^2-ad)\sin kl\right]\,, \quad \mathrm{e}^{i\varphi} = \frac{|c|}{\bar{c}}\,.$$

Clearly, λ_0 is real for real k, likewise, it is real also for pure imaginary $k = i\kappa$ because of

$$\lambda_0 = \frac{1}{2|c|\kappa}\left[-(a+d)\kappa\cosh\kappa l + (-\kappa^2 + |c|^2 - ad)\sinh\kappa l\right] .$$

The values of $|\lambda_+|$ and $|\lambda_-|$ depending on the values of λ_0 are shown in the table 5.1.

λ_0	$\lvert\lambda_+\rvert$	$\lvert\lambda_-\rvert$
$(-\infty, -1)$	< 1	> 1
$[-1, 1]$	1	1
$(1, \infty)$	> 1	< 1

Table 5.1: The values of $|\lambda_+|$ and $|\lambda_-|$ depending on λ_0

Furthermore, for real λ_0 one obtains

$$\lambda_+\bar{\lambda}_- = \mathrm{e}^{i\varphi}\left(\lambda_0 + \sqrt{\lambda_0^2 - 1}\right)\mathrm{e}^{-i\varphi}\left(\lambda_0 - \sqrt{\lambda_0^2 - 1}\right) = 1 .$$

We substitute the expression of A_j and B_j to (5.18) and study the coefficients of the terms $\sum_{j=0}^{\infty}|\lambda_+|^{2j}$, $\sum_{j=0}^{\infty}|\lambda_-|^{2j}$ and $\sum_{j=0}^{\infty}(\lambda_+^j\bar{\lambda}_-^j)$.

First, we express the coefficients of the unitary matrix U. The coefficients of the matrix $2\bar{c}k(M - \lambda_\pm\,\mathrm{id})$ are

$$\begin{aligned}
2\bar{c}k(M - \lambda_\pm\,\mathrm{id})_{11} &= (d-a)k\cos kl + (|c|^2 - ad - k^2)\sin kl \mp \sqrt{D}\,,\\
2\bar{c}k(M - \lambda_\pm\,\mathrm{id})_{12} &= 2ak\sin kl + 2(|c|^2 - ad)\cos kl\,,\\
2\bar{c}k(M - \lambda_\pm\,\mathrm{id})_{21} &= -2k^2\cos kl - 2dk\sin kl\,,\\
2\bar{c}k(M - \lambda_\pm\,\mathrm{id})_{22} &= -k(d-a)\cos kl - (|c|^2 - ad - k^2)\sin kl \mp \sqrt{D}\,,
\end{aligned}$$

where $D = [-(a+d)k\cos kl + (k^2 + |c|^2 - ad)\sin kl]^2 - 4|c|^2k^2$ means the discriminant and id unit 2x2 matrix. The eigenvectors of the matrix $M(k, \mathcal{A})$ can be chosen as

$$v_\pm = \begin{pmatrix} \frac{1}{N_\pm}v_1 \\ \frac{1}{N_\pm}v_{2\pm} \end{pmatrix} = \frac{1}{N_\pm}\begin{pmatrix} 2ak\sin kl + 2(|c|^2 - ad)\cos kl \\ (a-d)k\cos kl + (k^2 - |c|^2 + ad)\sin kl \pm \sqrt{D} \end{pmatrix} ,$$

where

$$\begin{aligned}
\frac{N_\pm^2}{2} &= 2[ak\sin kl + (|c|^2 - ad)\cos kl]^2 + (k^2\sin kl - dk\cos kl)^2 + \\
&[(|c|^2 - ad)\sin kl - ak\cos kl]^2 - 2|c|^2k^2 \pm [(a-d)k\cos kl + (k^2 - |c|^2 + ad)\sin kl]\cdot \\
&\cdot\sqrt{[-(a+d)k\cos kl + (k^2 + |c|^2 - ad)\sin kl]^2 - 4|c|^2k^2}\,.
\end{aligned}$$

The unitary matrix U is

$$U = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} = \begin{pmatrix} \frac{1}{N_+}\bar{v}_1 & \frac{1}{N_+}\bar{v}_{2+} \\ \frac{1}{N_-}\bar{v}_1 & \frac{1}{N_-}\bar{v}_{2-} \end{pmatrix} .$$

The terms in (5.18) can be rewritten using the coefficients of this matrix

$$A_j = A(\lambda_+ u_{12}\bar{u}_{11} + \lambda_- u_{22}\bar{u}_{21}) ,$$

$$B_j = A(\lambda_+ |u_{12}|^2 + \lambda_- |u_{22}|^2 ,$$

$$\sum_{j=1}^{\infty} |A_j|^2 = \sum_{j=0}^{\infty} [|\lambda_+|^{2j}|u_{11}|^2|u_{12}|^2 + \\ + |\lambda_-|^{2j}|u_{21}|^2|u_{22}|^2 + (\lambda_+^j \bar{\lambda}_-^j \bar{u}_{11}u_{12}u_{21}\bar{u}_{21} + \text{c.c.})] ,$$

$$\sum_{j=1}^{\infty} |B_j|^2 = \sum_{j=0}^{\infty} [|\lambda_+|^{2j}|u_{12}|^4 + |\lambda_-|^{2j}|u_{22}|^4 + (\lambda_+^j \bar{\lambda}_-^j |u_{11}|^2|u_{21}|^2 + \text{c.c.})] ,$$

$$\sum_{j=1}^{\infty} (A_j \bar{B}_j + \bar{A}_j B_j) = \sum_{j=0}^{\infty} \{|\lambda_+|^{2j}|u_{11}|^2(u_{11}\bar{u}_{12} + \bar{u}_{11}u_{12}) + \\ + |\lambda_-|^{2j}|u_{21}|^2(u_{21}\bar{u}_{22} + \bar{u}_{21}u_{22}) + [\lambda_+^j \bar{\lambda}_-^j (|u_{11}|^2 u_{21}\bar{u}_{22} + |u_{21}|^2 \bar{u}_{11}u_{12}) + \text{c.c.}]\} ,$$

where c. c. means the term complex conjugated to the previous one.

The norm of the wavefunction becomes

$$4k\|y\|^2 = [(4k^2l^2 - \sin 2kl)|u_{11}|^4 + (4k^2l^2 + \sin 2kl)|u_{11}|^2|u_{12}|^2 - \\ - \cos 2kl|u_{11}|^2(\bar{u}_{11}u_{12} + u_{11}\bar{u}_{12})] \sum_{j=0}^{\infty} |\lambda_+|^{2j} + [(4k^2l^2 - \sin 2kl)|u_{21}|^4 + \\ + (4k^2l^2 + \sin 2kl)|u_{21}|^2|u_{22}|^2 - \cos 2kl|u_{21}|^2(u_{21}\bar{u}_{22} + \bar{u}_{21}u_{22})] \sum_{j=0}^{\infty} |\lambda_-|^{2j} + \\ + [(4k^2l^2 - \sin 2kl)|u_{11}|^2|u_{21}|^2 + (4k^2l^2 + \sin 2kl)u_{11}\bar{u}_{21}\bar{u}_{12}u_{22} - \\ - \cos 2kl(|u_{11}|^2 u_{22}\bar{u}_{21} + |u_{21}|^2 u_{11}\bar{u}_{12})] \sum_{j=0}^{\infty} \lambda_+^j \bar{\lambda}_-^j + \text{c.c.} . \quad (5.19)$$

We can use also the parametrization (5.5) – (5.6). We obtain

$$\lambda_0 = \frac{(4 + \det \mathcal{A}_\mathrm{h}) \cos kl + \frac{2}{k}(\alpha_\mathrm{h} - \beta_\mathrm{h} k^2) \sin kl}{\sqrt{(4 - \det \mathcal{A}_\mathrm{h})^2 + (4 \operatorname{Im} \gamma_\mathrm{h})^2}}, \tag{5.20}$$

and the roots of the quadratic equation are

$$\lambda_\pm = \frac{1}{k(4 - \det \mathcal{A}_\mathrm{h} - 4i \operatorname{Im} \gamma_\mathrm{h})} \left[(4 + \det \mathcal{A}_\mathrm{h}) \cos kl + \frac{2}{k}(\alpha_\mathrm{h} - \beta_\mathrm{h} k^2) \sin kl \pm \sqrt{D} \right],$$

where

$$D = [(4 + \det \mathcal{A}_\mathrm{h}) k \cos kl + 2(\alpha - \beta k^2) \sin kl]^2 - k^2 [(4 + \det \mathcal{A}_\mathrm{h})^2 + (4 \operatorname{Im} \gamma_\mathrm{h})^2].$$

The eigenvectors of the matrix M could be chosen as

$$v_\pm = \frac{1}{N_\pm} \begin{pmatrix} v_{1\pm} \\ v_2 \end{pmatrix} = \frac{1}{N_\pm} \begin{pmatrix} 4 \operatorname{Re} \gamma_\mathrm{h} \cos kl + 2(\alpha_\mathrm{h} + \beta_\mathrm{h} k^2) \sin kl \pm \sqrt{D} \\ 4\beta k^2 \cos kl + (4 + \det \mathcal{A}_\mathrm{h} - 4 \operatorname{Re} \gamma_\mathrm{h}) k \sin kl \end{pmatrix}.$$

Notice that the case $|\lambda_+| = |\lambda_-| = 1$, i. e., $\lambda_0 \in [-1, 1]$ corresponds to the essential spectrum. From the form (5.20) we obtain the condition for the essential spectrum (5.16) again.

The point spectrum of the operator $\mathbf{H}_0$ consists of all the k for which (5.19) is finite. We must set the coefficient by $\sum_{j=0}^{\infty} \lambda_+^j \lambda_-^j$ and one of the coefficients by $\sum_{j=0}^{\infty} |\lambda_\pm|^{2j}$ to be zero. Moreover, the other sum must be finite and λ_0 must satisfy the corresponding inequation according to the table 5.1. For example, the norm is finite for $v_{2+} = 0$ and $\lambda_0 > 1$ or for the combination $v_{1-} = 0$ and $\lambda_0 < -1$.

5.5.3 The spectrum of the operator $\mathbf{H}_0$

The essential spectrum of the operator $\mathbf{H}_0(\mathcal{A}_\mathrm{t}, l)$ is given by the theorems 5.1 and 5.3 and lemma 5.7.

Theorem 5.4. *Let us assume the operator $\mathbf{H}_0(\mathcal{A}_\mathrm{t}, l)$ with non-separating conditions, i.e. $\det \mathcal{A}_\mathrm{h} \neq 4$ or $\operatorname{Im} \gamma \neq 0$. Its essential spectrum is given by the bands described in theorem 5.3 of multiplicity $b_0 \dots b_{n-1}(b_n - 1) + 1$. The cases described in theorem 5.3 correspond to*

a) $\beta_\mathrm{t} \neq 0$,

b) $\beta_\mathrm{t} = 0$ *and* $4(b+1) \operatorname{Re} \gamma_\mathrm{t} \neq (b-1)(4 + |\gamma_\mathrm{t}|)^2$,

c) $\beta_\mathrm{t} = 0$ *and* $4(b+1) \operatorname{Re} \gamma_\mathrm{t} = (b-1)(4 + |\gamma_\mathrm{t}|)^2)$.

The condition

d) $\alpha_{\rm t}=0$, $\beta_{\rm t}=0$, $\mathrm{Im}\,\gamma_{\rm t}=0$, *and* $(b-1)\mathrm{Re}\,\gamma_{\rm t}=2(\sqrt{b}\pm 1)^2$

implies the free coupling conditions on the halfline, i.e. the spectrum $[0,\infty)$.

Proof. The proof follows from the theorems 5.1 and 5.3 and lemma 5.7. The correspondence of the cases is given by the lemma 5.2. The case d) follows from the lemma 5.2, we require $\alpha_{\rm h}=\beta_{\rm h}=\gamma_{\rm h}=0$. □

Theorem 5.5. *The point spectrum of the operator* $\mathbf{H}_0(\mathcal{A}_{\rm t},l)$ *consists of* $\epsilon=k^2$, *where* k *satisfies the condition 1) and one of the conditions 2A) and 2B). All the points have infinite multiplicity.*

1)

$$[(4k^2l^2-\sin 2kl)|u_{11}|^2|u_{21}|^2+(4k^2l^2+\sin 2kl)u_{11}\bar{u}_{21}\bar{u}_{12}u_{22}-$$
$$-\cos 2kl(|u_{11}|^2u_{22}\bar{u}_{21}+|u_{21}|^2u_{11}\bar{u}_{12})]+\text{c.c.}=0\,,$$

2A)

$$(4k^2l^2-\sin 2kl)|u_{11}|^4+(4k^2l^2+\sin 2kl)|u_{11}|^2|u_{12}|^2-$$
$$-\cos 2kl|u_{11}|^2(\bar{u}_{11}u_{12}+u_{11}\bar{u}_{12})=0\,,\quad\text{and}\quad\lambda_0\in(1,\infty)\,,$$

2B)

$$(4k^2l^2-\sin 2kl)|u_{21}|^4+(4k^2l^2+\sin 2kl)|u_{21}|^2|u_{22}|^2-$$
$$-\cos 2kl|u_{21}|^2(u_{21}\bar{u}_{22}+\bar{u}_{21}u_{22})=0\,,\quad\text{and}\quad\lambda_0\in(-\infty,-1)\,,$$

2C)

$$(4k^2l^2-\sin 2kl)(|u_{21}|^4+|u_{11}|^4)+(4k^2l^2+\sin 2kl)(|u_{21}|^2|u_{22}|^2+|u_{11}|^2|u_{12}|^2)-$$
$$-\cos 2kl[|u_{21}|^2(u_{21}\bar{u}_{22}+\bar{u}_{21}u_{22})+|u_{11}|^2(\bar{u}_{11}u_{12}+u_{11}\bar{u}_{12})]=0\,,$$

where

$$u_{11}=\frac{1}{N_+}[4\,\mathrm{Re}\,\gamma_{\rm h}\cos kl+2(\alpha_{\rm h}+\beta_{\rm h}k^2)\sin kl+\sqrt{D}]\,,$$
$$u_{12}=\frac{1}{N_+}[4\beta k^2\cos kl+(4+\det\mathcal{A}_{\rm h}-4\,\mathrm{Re}\,\gamma_{\rm h})k\sin kl\,,$$
$$u_{21}=\frac{1}{N_-}[4\,\mathrm{Re}\,\gamma_{\rm h}\cos kl+2(\alpha_{\rm h}+\beta_{\rm h}k^2)\sin kl-\sqrt{D}]\,,$$
$$u_{22}=\frac{1}{N_-}[4\beta k^2\cos kl+(4+\det\mathcal{A}_{\rm h}-4\,\mathrm{Re}\,\gamma_{\rm h})k\sin kl\,,$$

$$D=[(4+\det\mathcal{A}_{\rm h})\;\;k\;\;\cos kl+2(\alpha-\beta k^2)\sin kl]^2-k^2[(4+\det\mathcal{A}_{\rm h})^2+(4\,\mathrm{Im}\,\gamma_{\rm h})^2]\,.$$

Notice that the sufficient conditions for the point spectrum of the operator $\mathbf{H}_0(\mathcal{A}_{\mathrm{t}}, l)$ are

$$u_{11} = 0 \quad \text{and} \qquad \text{and} \quad \lambda_0 \in (1, \infty)\,,$$

or

$$u_{21} = 0 \quad \text{and} \qquad \text{and} \quad \lambda_0 \in (-\infty, -1)\,,$$

or

$$u_{11} = 0 \quad \text{and} \qquad \text{and} \quad u_{21} = 0\,.$$

The free conditions (the case discussed in [SS02]) give $u_{11} = 4ik \sin kl$ and $u_{21} = -4ik \sin kl$, hence the eigenvalues $kl = n\pi$ are present.

Chapter 6

Conclusions

We have studied several problems concerning quantum graphs. In two concrete examples of quantum graphs we have found trajectories of poles of the resolvent when lengths of the edges were perturbed. The main result of the first part of the work states that the embedded eigenvalue in the unperturbed spectrum of multiplicity n gives raise to n resonances.

In the next section we have investigated the spectral manifold of star graphs. We have slightly generalized Cheon's, Fülöp's and Tsutsui's result ([CFT01b]) by describing the spectral manifold of a star graph with two edges with different lengths. Furthermore, we have studied Berry's phase for a larger class of quantum graphs then in [EG99] and we have demonstrated that Berry's phase can take any value in $[0, 2\pi)$.

The last part of the work was devoted to tree graphs. We have generalized Sobolev's and Solomyak's result ([SS02]) by investigating the unitary equivalence between the Hamiltonian on tree graph and the sum of Hamiltonians on $L^2(\mathbb{R}_+)$. We have studied the spectrum for a more concrete case.

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