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BAKALÁŘSKÁ PRÁCE

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Rezonance v kvantových grafech

Ústav teoretické fyziky

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BACHELOR THESIS

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Resonances in quantum graphs

Institute of Theoretical Physics

Supervisor: Prof. RNDr. Pavel Exner, DrSc.,
Doppler Institute, Czech Technical University
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Prohlašuji, že jsem svou bakalářskou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce a jejím zveřejňováním.

V Praze dne 25. 5. 2006 Jiří Lipovský

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Abstrakt: V této práci studujeme diferenciální operátor druhého řádu na grafu s několika připojenými polopřímkami. Nejdříve popíšeme základní vlastnosti kvantových grafů a metodu komplexního škálování. Na jednoduchých konkrétních příkladech uvedeme použití této metody a porovnáme získané rezonanční póly s póly matice rozptylu. V obecném případě ověříme samoadjungovanost uvažovaného hamiltoniánu na grafu s konkrétními vazebnými podmínkami. Potom použijeme metodu popsanou na příkladech a nalezneme soustavu rovnic pro rezonanční póly. Dokážeme, že odpovídá soustavě rovnic pro póly matice rozptylu.

Klíčová slova: kvantové grafy, komplexní škálování, rozptyl, mezoskopické systémy

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Abstract: In the present work we study a second-order differential operator on a graph with some attached semiinfinite links. First, we describe basic properties of the quantum graphs and the method of complex scaling. In simple particular examples we show using this method and compare the obtained resonance poles with poles of the scattering matrix. In the general case we verify the selfadjoitness of the considered Hamiltonian on the graph with particular coupling conditions. Then we use the method described in the examples and find the system of equations for resonance poles. We prove that it corresponds to the system of equations for poles of the scattering matrix.

Keywords: quantum graphs, complex scaling, scattering, mesoscopic systems

Chapter 1

Introduction

We consider a planar graph equipped by a selfadjoint second-order differential operator; the aim is to study the motion of a quantum particle on this configuration space.

A motivation for this problem comes from the fact that such a graph can model small semiconductor structure, often under influence of an electric or magnetic field, and similar systems based on metals or carbon nanotubes. The model description can predict conductance and other quantum effects.

Such structures are called a quantum wire, the quantum particle (electron) moves within the wire. Quantum wires and their properties has been described e. g. in [3], [6] or [11].

We restrict our attention to the idealized model, usually called quantum graph, in which the wire width is neglected. A summary on quantum graphs can be found in [4], [9] or [10], particular examples are in [5], [7] or [8].

We will study the scattering problem on graphs, in particular, the question about resonances in such systems. They are usually determined through poles of the on-shell scattering matrix (S-matrix). In the theory of Schrödinger operators, however, one often uses an alternative approach based on the method of so-called complex scaling, whose idea is due to Aguilar and Combes – see, e.g., [1] or [12].

We will apply this method to graph scattering and derive equations which allow us to determine poles of the graph Hamiltonian resolvent. In particular, we will show that they coincide with those of the scattering matrix.

Chapter 2

Description of the model

Let us consider a graph Γ consisting of finite or countable number of vertices $\mathcal{X}_j, j \in I$ where I is a index set. We denote this set of vertices $\mathcal{V} = \{\mathcal{X}_j, j \in I\}$, the set of neighbours $\mathcal{X}_j$ we denote $\mathcal{N}(\mathcal{X}_j) = \{\mathcal{X}_n : n \in \nu(j) \subset I \backslash \{j\}\}$. Each edge with finite length can be identified by a pair of vertices. The set of finite edges is $\mathcal{L} = \{\mathcal{L}_{jn} : (\mathcal{X}_j, \mathcal{X}_n) \in I_{\mathcal{L}} \subset I \times I\}$. Length l_{jn} of each edge in $\mathcal{L}$ is positive. To some vertices in $\mathcal{V}$ we attach one semiinfinite link. The union of these links and the graph Γ we denote by Γ_e.

We denote by $\mathcal{B}$ the set of vertices which have a single neighbour, graph interior is $\mathcal{I} = \mathcal{V} \backslash \mathcal{B}$. We denote by $\mathcal{C}$ the set of vertices to which is attached a semiinfinite link. Similarly, we denote by $I_{\mathcal{B}}$, $I_{\mathcal{I}}$, and $I_{\mathcal{C}}$ the index subsets in I.

The metric on the graph can be indentified with a part of a Euclidean space. The considered Hilbert space is

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

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

Furthermore, we define on the graph Γ_e the diferential operator $H = \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)$ with essentially bounded potential $V = \{V_{jn}, V_{j\infty}\}, V_{jn} \in L^\infty([0, l_{jn}]), V_{j\infty} = 0$. This is the Hamiltonian of the quantum particle, for simplicity we set the coefficient $\hbar^2/2m$ in Schrödinger equation equal to 1. The domain of definition of this Hamiltonian are functions ψ in 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 correspond to the coupling condition.

We denote the limits of functions and their derivatives on $\mathcal{L}_{jn}$ (the point $\mathcal{X}_j$ is identified with $x = 0$)

$$\psi_{jn} = \lim_{x\to 0+} \psi_{jn}(x),$$

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

On each vertex $\mathcal{X}_j$ we denote

$$\Psi = (\psi_1(\mathcal{X}_j), \psi_2(\mathcal{X}_j), \dots, \psi_d(\mathcal{X}_j))^T, \quad d = \mathrm{card}\,\mathcal{N}_j$$

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

$$\Psi' = (\psi'_1(\mathcal{X}_j), \psi'_2(\mathcal{X}_j), \dots, \psi'_d(\mathcal{X}_j))^T, \quad d = \mathrm{card}\,\mathcal{N}_j$$

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

The general coupling condition at the vertex $\mathcal{X}_j$ is

$$A_{\mathcal{X}_j}\Psi + B_{\mathcal{X}_j}\Psi' = 0,$$

here $A_{\mathcal{X}_j}$ and $B_{\mathcal{X}_j}$ are matrices of rank d. In lemma 2.2 in [9] is proven that for matrices $A_{\mathcal{X}_j}$, $B_{\mathcal{X}_j}$ such that (A, B) has maximal rank the Hamiltonian H is selfadjoint if and only if the matrix $A_{\mathcal{X}_j}{B_{\mathcal{X}_j}}^\dagger$ is selfadjoint at each vertex.

In particular, there are two special possibilities of coupling

1. δ-coupling:

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

2. δ'-coupling:

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

Chapter 3

Complex scaling

On a fixed halfline let us consider scaling transformation $g_\vartheta = U_\vartheta g(x) = \mathrm{e}^{\vartheta/2} g(x\,\mathrm{e}^{\vartheta})$ with complex parameter ϑ. We may demonstrate the transformation of the free motion Hamiltonian on a halfline by the action on a function g.

$$\begin{aligned} H_\vartheta g(x) &= U_\vartheta H U_\vartheta^{-1} g(x) = U_\vartheta H\,\mathrm{e}^{-\vartheta/2} g(x\,\mathrm{e}^{-\vartheta}) = -\,\mathrm{e}^{-\vartheta/2} U_\vartheta [g(x\,\mathrm{e}^{-\vartheta})]'' = \\ &= -\,\mathrm{e}^{-\vartheta/2}\,\mathrm{e}^{-2\vartheta} U_\vartheta g''(x\,\mathrm{e}^{-\vartheta}) = -\,\mathrm{e}^{-\vartheta/2}\,\mathrm{e}^{\vartheta/2}\,\mathrm{e}^{-2\vartheta} g''(x) = \,\mathrm{e}^{-2\vartheta} H g(x). \end{aligned}$$

This means that the Hamiltonian is transformed as follows

$$H_\vartheta = U_\vartheta H U_\vartheta^{-1} = -\,\mathrm{e}^{-2\vartheta}\Delta.$$

The domain of definition of the transformed Hamiltonian is $D(H_\vartheta) = U_\vartheta D(H)$, it consists of functions $g_\vartheta = U_\vartheta g$.

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 essentially bounded. We use the mentioned transformation on the external edges. The transformed Hamiltonian is

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

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 domain of definition of the transformed Hamiltonian consists of functions with components $f_{jn} \in W^{2,2}([0, l_{jn}])$ and $g_{j\vartheta} = U_\vartheta g_j$ satisfying the coupling conditions.

The solution of the Schrödinger equation on the halfline $g_{j\vartheta}$ can be expressed as a linear combination of functions

$$\begin{aligned}\psi_+ &= \mathrm{e}^{\mathrm{i}kx\,\mathrm{e}^{\vartheta}},\\ \psi_- &= \mathrm{e}^{-\mathrm{i}kx\,\mathrm{e}^{\vartheta}}.\end{aligned}$$

Now we find when $\psi_+ \in L^2(\mathbb{R}^+)$. We denote the real and the imaginary part of k by k_r and k_i, respectively.

$$\psi_+ = \mathrm{e}^{\mathrm{i}x(k_\mathrm{r}+\mathrm{i}k_\mathrm{i})\,\mathrm{e}^{\vartheta_\mathrm{r}}(\cos\vartheta_\mathrm{i}+\mathrm{i}\sin\vartheta_\mathrm{i})} = \mathrm{e}^{[\mathrm{i}x(k_\mathrm{r}\cos\vartheta_\mathrm{i}-k_\mathrm{i}\sin\vartheta_\mathrm{i})-x(k_\mathrm{i}\cos\vartheta_\mathrm{i}+k_\mathrm{r}\sin\vartheta_\mathrm{i})]\,\mathrm{e}^{\vartheta_\mathrm{r}}}.$$

For $\vartheta_\mathrm{i} \in (0, \pi/2)$ is $\sin\vartheta_\mathrm{i} > 0$, $\cos\vartheta_\mathrm{i} > 0$, and for $k_\mathrm{r} > 0$, $k_\mathrm{i} < 0$ is the term $k_\mathrm{i}\cos\vartheta_\mathrm{i} + k_\mathrm{r}\sin\vartheta_\mathrm{i}$ non-negative if $\tan\vartheta_\mathrm{i} \geq |k_\mathrm{i}/k_\mathrm{r}|$, the solution $\psi_+ \in L^2(\mathbb{R}^+)$. For ψ_- we proceed similarly.

For the internal edges we find the solutions of the Schrödinger equation as a linear combination of $\mathrm{e}^{\mathrm{i}kx}$ and $\mathrm{e}^{-\mathrm{i}kx}$. We choose the coefficients of this combination according to the coupling conditions.

Chapter 4

Examples

4.1 Example 1 – A line with an appendix

We consider a line connected at the point $x = 0$ to an appedix of length $l > 0$. The Hilbert space is $L^2(\mathbb{R}) \bigoplus L^2([0, l])$, i. e. state is described by $\psi = \binom{g}{f}$ where the component g refers to the line and the component f to the appendix (see Figure 4.1). The Hamiltonian is defined by

$$H\psi = \begin{pmatrix} -g'' \\ -f'' \end{pmatrix}.$$

At the point $x = 0$ we consider the same coupling condition as in [8], at the other end of the appendix the condition $f(l) = 0$.

$$\begin{aligned} g(0) &:= g(0+) = g(0-), \\ f(0) &= bg(0) + cf'(0), \\ g'(0+) - g'(0-) &= dg(0) - bf'(0), \\ f(l) &= 0. \end{aligned}$$

First, we solve the scattering problem, in the way used in [8]. From the left there goes a wave $\mathrm{e}^{\mathrm{i}kx}$, reflected wave is $r\,\mathrm{e}^{-\mathrm{i}kx}$ and transmitted wave $t\mathrm{e}^{\mathrm{i}kx}$. After substituting we get following system of equations.

$$t = 1 + r, \tag{4.1}$$

$$f(0) = bt + cf'(0), \tag{4.2}$$

$$\mathrm{i}k(t - 1 + r) = dt - bf'(0), \tag{4.3}$$

$$f(l) = 0. \tag{4.4}$$

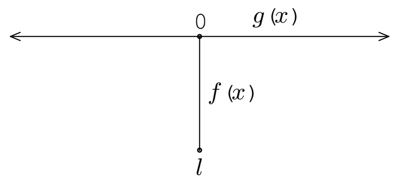

Figure 4.1: Example 1

If $f_l(x)$ solves Schrödinger equation at the appendix and satisfies condition $f_l(l) = 0$ we can express the solution $f(x)$ as a multiple of this function, $f(x) = \beta f_l(x)$. The constant β can be easily obtained from the equation (4.2).

$$\beta = \frac{bt}{f_l(0) - cf_l'(0)}.$$

After substituting into (4.1) and (4.3) we get as in [8]

$$2ikr = (1+r)\left(d - \frac{b^2 f_l'(0)}{f_l(0) - cf_l'(0)}\right),$$

$$r = \frac{d[f_l(0) - cf_l'(0)] - b^2 f_l'(0)}{(2ik - d)[f_l(0) - cf_l'(0)] + b^2 f_l'(0)}, \tag{4.5}$$

$$t = \frac{2ik[f_l(0) - cf_l'(0)]}{(2ik - d)[f_l(0) - cf_l'(0)] + b^2 f_l'(0)}. \tag{4.6}$$

In particular, choosing $b = 1$ and $c = 0$ we can simplify the coupling condition and get the δ-coupling with the parameter $\alpha = d$. Equations (4.5) and (4.6) then become

$$r = \frac{df_l(0) - f_l'(0)}{(2ik - d)f_l(0) + f_l'(0)},$$

$$t = \frac{2ikf_l(0)}{(2ik - d)f_l(0) + f_l'(0)}.$$

Studying transmission and reflection coefficients $\tilde{t}$, $\tilde{r}$ for the wave going from the right we get the same system of equations as in (4.1) – (4.4), solution is same.

We can find poles of the S-matrix by finding when the denominator of both fractions is zero. We obtain the condition

$$(2ik - d)[f_l(0) - cf_l'(0)] + b^2 f_l'(0) = 0,$$

where $f_l(x)$ is the solution of Schrödinger equation satisfying $f_l(l) = 0$.

We can choose $f_l(x) = \sin k(l - x)$, we get the equation

$$(2\mathrm{i}k - d)(\sin kl + ck\cos kl) - b^2 k\cos kl = 0,$$

hence we obtain the equation for resonances

$$\tan kl = \frac{b^2 k}{2\mathrm{i}k - d} - ck.$$

Now we try to find the positions of the resonance poles by studying the singularities of the resolvent. We use the introduced method of complex scaling. Let us scale functions on both infinite edges by transformation $g_\vartheta(x) = \mathrm{e}^{\vartheta/2} g(\mathrm{e}^\vartheta x)$. We obtain

$$\begin{aligned}
g'_\vartheta(x) &= \mathrm{e}^{3\vartheta/2} g(\mathrm{e}^\vartheta x), \\
g_\vartheta(0) &= \mathrm{e}^{\vartheta/2} g(0), \\
g_\vartheta(x) &= g_\vartheta(0)\mathrm{e}^{\mathrm{i}kx\,\mathrm{e}^\vartheta}, \qquad x \in \mathbb{R}^+, \\
g_\vartheta(x) &= g_\vartheta(0)\,\mathrm{e}^{-\mathrm{i}kx\,\mathrm{e}^\vartheta}, \quad x \in \mathbb{R}^-, \\
g'_\vartheta(0+) &= \mathrm{i}k\,\mathrm{e}^\vartheta g_\vartheta(0), \qquad (4.7) \\
g'_\vartheta(0-) &= -\mathrm{i}k\,\mathrm{e}^\vartheta g_\vartheta(0). \qquad (4.8)
\end{aligned}$$

Substituting into boundary conditions we get

$$\begin{aligned}
1 + r &= t, \qquad (4.9) \\
f(0) &= b\,\mathrm{e}^{-\vartheta/2} g_\vartheta(0) + cf'(0), \qquad (4.10) \\
\mathrm{e}^{-3\vartheta/2}[g'_\vartheta(0+) - g'_\vartheta(0-)] &= d\,\mathrm{e}^{-\vartheta/2}(0) g_\vartheta(0) - bf'(0), \qquad (4.11) \\
f(l) &= 0.
\end{aligned}$$

The solution on the appendix can be expressed as $f(x) = \beta\sin k(l - x)$. From (4.10) we obtain

$$\beta = \frac{b\,\mathrm{e}^{-\vartheta/2}}{\sin kl + ck\cos kl}\, g_\vartheta(0),$$

substituting it into (4.11) and using (4.7) and (4.8) we get

$$\mathrm{e}^{-3\vartheta/2} g_\vartheta(0) 2\mathrm{i}k\,\mathrm{e}^\vartheta = g_\vartheta(0)\,\mathrm{e}^{-\vartheta/2}\left[d - \frac{b^2(-k\cos kl)}{\sin kl + ck\cos kl}\right].$$

That gives the same condition for poles

$$\tan kl = \frac{b^2 k}{2\mathrm{i}k - d} - ck.$$

We conclude that the equation for resonance poles obtained by complex scaling is the same as the equation for poles of the S-matrix.

For $c = d = 0$ we can exactly solve the equation; we express $\tan kl$ as a combination of complex exponentials

$$\frac{\mathrm{e}^{\mathrm{i}kl} - \mathrm{e}^{-\mathrm{i}kl}}{\mathrm{i}(\mathrm{e}^{\mathrm{i}kl} + \mathrm{e}^{-\mathrm{i}kl})} = \frac{b^2}{2\mathrm{i}},$$

we obtain the equation

$$\left(1 - \frac{b^2}{2}\right)(\mathrm{e}^{\mathrm{i}kl})^2 - \left(\frac{b^2}{2} + 1\right) = 0,$$

for $|b| \neq \sqrt{2}$ we have $\mathrm{e}^{2\mathrm{i}kl} = (b^2+2)/(2-b^2)$ and similarly to [8] we obtain

$$k_n = \frac{n\pi}{l} + \frac{\mathrm{i}}{2l}\ln\frac{2-b^2}{2+b^2}, \qquad |b| < \sqrt{2},$$

$$k_n = \frac{\pi}{2l} + \frac{n\pi}{l} + \frac{\mathrm{i}}{2l}\ln\frac{b^2-2}{2+b^2}, \qquad |b| > \sqrt{2}.$$

For $|b| = \sqrt{2}$ we cannot satisfy the equation (4.1) for any k, there are no resonance poles.

4.2 Example 2 – Two internal edges

Let us consider a graph consisting of two internal edges of length l_1 and l_2, respectively, which are connected at both ends with two added halflines (see Figure 4.2). The Hilbert space is $L^2(\mathbb{R}^-) \bigoplus L^2(\mathbb{R}^+) \bigoplus L^2([0,l_1]) \bigoplus L^2([0,l_2])$, state is described by the column

$$\psi = \begin{pmatrix} f \\ g \\ u \\ v \end{pmatrix}.$$

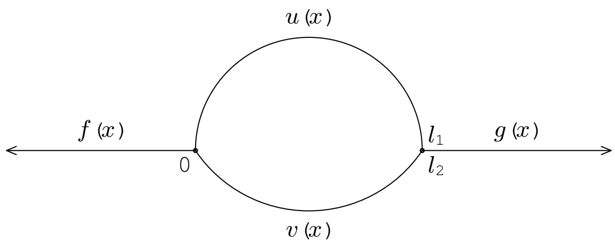

Figure 4.2: Example 2

The Hamiltonian is defined by

$$H\psi = \begin{pmatrix} -f'' \\ -g'' \\ -u'' \\ -v'' \end{pmatrix}.$$

We start by finding the poles of the S-matrix again. From the left there goes a wave $\mathrm{e}^{\mathrm{i}kx}$, transmission amplitude is t and reflection amplitude r. We define functions at both halflines

$$\begin{aligned} f &= \mathrm{e}^{\mathrm{i}kx} + r\,\mathrm{e}^{-\mathrm{i}kx}, \qquad && x \in (-\infty, 0], \\ g &= t\mathrm{e}^{\mathrm{i}kx}, && x \in [0, \infty), \end{aligned}$$

on the internal edges we define functions u and v.

Let us consider δ-conditions at both vertices, i. e.,

$$u(0) = v(0) = f(0) = 1 + r,$$
$$u(l_1) = v(l_2) = g(0) = t,$$
$$u'(0) + v'(0) - f'(0) = \alpha f(0), \tag{4.12}$$
$$-u'(l_1) - v'(l_2) + g'(0) = \beta g(0). \tag{4.13}$$

The lhs of (4.12) and (4.13) are sums of outward derivatives, that gives the signs of the functions. We substitute functions f and g and their derivatives into (4.12) and (4.13).

$$u'(0) + v'(0) - \mathrm{i}k(1 - r) = \alpha(1 + r), \tag{4.14}$$
$$-u'(l_1) - v'(l_2) + t\mathrm{i}k = \beta t, \tag{4.15}$$

The solutions u and v can be expressed as a superposition of the waves $\mathrm{e}^{\mathrm{i}kx}$ and $\mathrm{e}^{-\mathrm{i}kx}$.

$$u = u_1 \mathrm{e}^{\mathrm{i}kx} + u_2\, \mathrm{e}^{-\mathrm{i}kx},$$
$$v = v_1 \mathrm{e}^{\mathrm{i}kx} + v_2\, \mathrm{e}^{-\mathrm{i}kx}.$$

Comparing these equations with boundary conditions for u we get

$$u(0) = u_1 + u_2 = 1 + r,$$
$$u(l_1) = u_1 \mathrm{e}^{\mathrm{i}kl_1} + u_2\, \mathrm{e}^{-\mathrm{i}kl_1} = t,$$

hence we obtain

$$u_1 = \frac{t - (1+r)\, \mathrm{e}^{-\mathrm{i}kl_1}}{\mathrm{e}^{\mathrm{i}kl_1} - \mathrm{e}^{-\mathrm{i}kl_1}},$$
$$u_2 = \frac{(1+r)\, \mathrm{e}^{\mathrm{i}kl_1} - t}{\mathrm{e}^{\mathrm{i}kl_1} - \mathrm{e}^{-\mathrm{i}kl_1}}.$$

It is not difficult to realise that for v we get same equations except that l_1 is replaced by l_2.

We compute derivatives of the function u at the endpoints

$$u'(0) = \mathrm{i}k(u_1 - u_2) = \frac{kt}{\sin kl_1} - \frac{k(1+r)}{\tan kl_1},$$
$$u'(l_1) = \mathrm{i}k(u_1 \mathrm{e}^{\mathrm{i}kl_1} - u_2\, \mathrm{e}^{-\mathrm{i}kl_1}) = \frac{kt}{\tan kl_1} - \frac{k(1+r)}{\sin kl_1},$$

for v the results are similar. Now we can rewrite the equations (4.14) and (4.15)

$$t\left(\frac{1}{\sin kl_1} + \frac{1}{\sin kl_2}\right) - (r+1)\left(\frac{1}{\tan kl_1} + \frac{1}{\tan kl_2}\right) - \mathrm{i}(1-r) = \\ = \frac{\alpha}{k}(1+r), \quad (4.16)$$

$$(1+r)\left(\frac{1}{\sin kl_1} + \frac{1}{\sin kl_2}\right) - t\left(\frac{1}{\tan kl_1} + \frac{1}{\tan kl_2}\right) + \mathrm{i}t = \frac{\beta}{k}t.$$

From the last equation we express

$$t = \frac{(1+r)\left(\frac{1}{\sin kl_1} + \frac{1}{\sin kl_2}\right)}{\frac{1}{\tan kl_1} + \frac{1}{\tan kl_2} + \frac{\beta}{k} - i},$$

substituting into (4.16) we obtain

$$(r+1)\left[\frac{\left(\frac{1}{\sin kl_1}+\frac{1}{\sin kl_2}\right)^2}{\frac{1}{\tan kl_1}+\frac{1}{\tan kl_2}+\frac{\beta}{k}-i}-\left(\frac{1}{\tan kl_1}+\frac{1}{\tan kl_2}\right)-\frac{\alpha}{k}\right]=-\mathrm{i}(r-1).$$

Denoting

$$\gamma(k)=\frac{\left(\frac{1}{\sin kl_1}+\frac{1}{\sin kl_2}\right)^2}{\frac{1}{\tan kl_1}+\frac{1}{\tan kl_2}+\frac{\beta}{k}-i}-\left(\frac{1}{\tan kl_1}+\frac{1}{\tan kl_2}\right)-\frac{\alpha}{k}$$

we can express reflection and transmission coefficients

$$r=\frac{\mathrm{i}-\gamma(k)}{\gamma(k)+\mathrm{i}},$$
$$t=\frac{2\mathrm{i}}{\gamma(k)+\mathrm{i}}.$$

The condition for poles of the scattering matrix is now

$$\frac{\left(\frac{1}{\sin kl_1}+\frac{1}{\sin kl_2}\right)^2}{\frac{1}{\tan kl_1}+\frac{1}{\tan kl_2}+\frac{\beta}{k}-\mathrm{i}}-\left(\frac{1}{\tan kl_1}+\frac{1}{\tan kl_2}\right)-\left(\frac{\alpha}{k}-\mathrm{i}\right)=0. \qquad (4.17)$$

Now we find the resonance poles by complex scaling. We scale both the halflines in the way similar to the example 1.

$$\begin{aligned}
f_\vartheta(x) &= \mathrm{e}^{\vartheta/2}f(x\,\mathrm{e}^{\vartheta}),\\
g_\vartheta(x) &= \mathrm{e}^{\vartheta/2}g(x\,\mathrm{e}^{\vartheta}),\\
f_\vartheta(0-) &= \mathrm{e}^{\vartheta/2}f(0-) = \mathrm{e}^{\vartheta/2}u(0) = \mathrm{e}^{\vartheta/2}v(0), && (4.18)\\
g_\vartheta(0+) &= \mathrm{e}^{\vartheta/2}g(0+) = \mathrm{e}^{\vartheta/2}u(l_1) = \mathrm{e}^{\vartheta/2}v(l_2). && (4.19)
\end{aligned}$$

The solution of Schrödinger equation on both halflines is

$$f_\vartheta(x)=f_\vartheta(0-)\psi_-=f_\vartheta(0-)\,\mathrm{e}^{-\mathrm{i}kx\,\mathrm{e}^{\vartheta}},$$
$$g_\vartheta(x)=g_\vartheta(0+)\psi_+=g_\vartheta(0+)\,\mathrm{e}^{\mathrm{i}kx\,\mathrm{e}^{\vartheta}},$$

derivatives at the point $x = 0$ are

$$\begin{aligned} f'_\vartheta(0-) &= -f_\vartheta(0-)\mathrm{i}k\,\mathrm{e}^{\vartheta} = \mathrm{e}^{3\vartheta/2} f'(0-),\\ g'_\vartheta(0+) &= g_\vartheta(0+)\mathrm{i}k\,\mathrm{e}^{\vartheta} = \mathrm{e}^{3\vartheta/2} g'(0+),\end{aligned}$$

Substituting into (4.12) and (4.13) we get the boundary conditions

$$\mathrm{i}k\,\mathrm{e}^{-\vartheta/2} f_\vartheta(0-) + u'(0) + v'(0) = \alpha\,\mathrm{e}^{-\vartheta/2} f_\vartheta(0-), \tag{4.20}$$

$$\mathrm{i}k\,\mathrm{e}^{-\vartheta/2} g_\vartheta(0+) - u'(l_1) - v'(l_2) = \beta\,\mathrm{e}^{-\vartheta/2} g_\vartheta(0+), \tag{4.21}$$

The solution of Schrödinger equation on finite edge satisfying the conditions (4.18) and (4.19) is

$$u(x) = \frac{f_\vartheta(0-)\sin k(l_1 - x) + g_\vartheta(0+)\sin kx}{\sin kl_1}\,\mathrm{e}^{-\vartheta/2},$$

its derivative is

$$u'(x) = \frac{-f_\vartheta(0-)\cos k(l_1 - x) + g_\vartheta(0+)\cos kx}{\sin kl_1} k\,\mathrm{e}^{-\vartheta/2},$$

For the function $v(x)$ satisfying the condition (4.19) we obtain similar equations (we only have to replace l_1 by l_2).

Substituting into (4.20) and (4.21) we get the equations

$$k\left[g_\vartheta(0+)\left(\frac{1}{\sin kl_1} + \frac{1}{\sin kl_2}\right) - f_\vartheta(0-)\left(\frac{1}{\tan kl_1} + \frac{1}{\tan kl_2}\right)\right] = \\ = (\alpha - \mathrm{i}k) f_\vartheta(0-), \tag{4.22}$$

$$k\left[g_\vartheta(0+)\left(\frac{1}{\tan kl_1} + \frac{1}{\tan kl_2}\right) - f_\vartheta(0-)\left(\frac{1}{\sin kl_1} + \frac{1}{\sin kl_2}\right)\right] = \\ = -(\beta - \mathrm{i}k) g_\vartheta(0+). \tag{4.23}$$

Hence we obtain the condition (4.17) again.

If both internal edges has the same length ($l = l_1 = l_2$) we can simplify this condition

$$\left(\frac{2}{\sin kl}\right)^2 - \left(\frac{2}{\tan kl}\right)^2 - \frac{2}{\tan kl}\left(\frac{\alpha+\beta}{k} - 2\mathrm{i}\right) - \left(\frac{\alpha}{k} - \mathrm{i}\right)\left(\frac{\beta}{k} - \mathrm{i}\right) = 0.$$

$$4 - \frac{2}{\tan kl}\left(\frac{\alpha+\beta}{k} - 2\mathrm{i}\right) - \left(\frac{\alpha}{k} - \mathrm{i}\right)\left(\frac{\beta}{k} - \mathrm{i}\right) = 0.$$

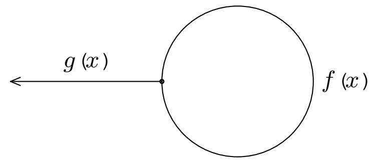

Figure 4.3: Lasso graph

For $\alpha = \beta = 0$ we obtain

$$5 \tan kl = -4\mathrm{i},$$
$$k = \frac{n\pi}{l} - \frac{\mathrm{i}\ln 9}{2l}.$$

4.3 Example 3 – Lasso graph

Let us consider a lasso-shaped graph on Figure 4.3, constisting of a loop of length l and a halfline. This type of the graph has been studied in [5]. The Hilbert space is $L^2(\mathbb{R}^+) \bigoplus L^2([0,l])$, state is described by $\psi = \binom{g}{f}$. The Hamiltonian is defined by

$$H\psi = \begin{pmatrix} -g'' \\ -f'' \end{pmatrix}.$$

We consider the following coupling (as in [5]) with parameters $\alpha, \tilde{\alpha} \in \mathbb{R}$ and $\gamma \in \mathbb{C}$. Choosing $\gamma = 0$ we can separate the halfline by switching the interaction between it and the loop off.

$$f(0) = f(l), \tag{4.24}$$
$$f(0) = \alpha^{-1}[f'(0) - f'(l)] + \gamma g'(0), \tag{4.25}$$
$$g(0) = \bar{\gamma}[f'(0) - f'(l)] + \tilde{\alpha}^{-1} g'(0). \tag{4.26}$$

The equation for the poles of the S-matrix is derived in [5], we only find the resonance poles by the metod of complex scaling. As in previous examples we scale the halfline

$$g_\vartheta(x) = \mathrm{e}^{\vartheta/2} g(\mathrm{e}^{\vartheta} x),$$
$$g_\vartheta(0) = \mathrm{e}^{\vartheta/2} g(0),$$
$$g'_\vartheta(0) = \mathrm{e}^{3\vartheta/2} g'(0).$$

We can easily find the solution f satisfying mentioned conditions.

$$\begin{aligned}
f(x) &= f(0)\frac{\sin kx + \sin k(l-x)}{\sin kl},\\
f'(x) &= kf(0)\frac{\cos kx - \cos k(l-x)}{\sin kl},\\
f'(0) &= kf(0)\frac{1-\cos kl}{\sin kl},\\
f'(l) &= kf(0)\frac{\cos kl - 1}{\sin kl}.
\end{aligned}$$

Substituting to (4.25) and (4.26) we obtain

$$f(0) = 2k\alpha^{-1}\frac{1-\cos kl}{\sin kl}f(0) + \gamma\,\mathrm{e}^{-3\vartheta/2}g'_\vartheta(0), \tag{4.27}$$

$$\mathrm{e}^{-\vartheta/2}g_\vartheta(0) = 2k\bar{\gamma}\frac{1-\cos kl}{\sin kl}f(0) + \tilde{\alpha}^{-1}\,\mathrm{e}^{-3\vartheta/2}g'_\vartheta(0). \tag{4.28}$$

On the halfline we take the solution $g_\vartheta(x) = \psi_+ = \mathrm{e}^{\mathrm{i}k\,\mathrm{e}^{\vartheta}}$. After substituting for $g'_\vartheta(0) = g_\vartheta(0)\mathrm{i}k\,\mathrm{e}^{\vartheta}$ into (4.28) we obtain

$$\begin{aligned}
f(0) &= 2k\alpha^{-1}\frac{1-\cos kl}{\sin kl}f(0) + \gamma\,\mathrm{e}^{-\vartheta/2}\mathrm{i}kg_\vartheta(0),\\
\mathrm{e}^{-\vartheta/2}g_\vartheta(0) &= 2k\bar{\gamma}\frac{1-\cos kl}{\sin kl}f(0) + \tilde{\alpha}^{-1}\mathrm{i}k\,\mathrm{e}^{-\vartheta/2}g_\vartheta(0).
\end{aligned}$$

From these two equations we get the condition

$$\frac{1}{2}\sin kl = \left(\frac{k}{\alpha} + \frac{\mathrm{i}|\gamma|^2k^2}{1-\tilde{\alpha}^{-1}\mathrm{i}k}\right)(1-\cos kl). \tag{4.29}$$

4.4 Example 4 – Lasso graph in a homogenous magnetic field

We consider the same graph as in previous example placed into a homogenous magnetic field perpendicular to the loop plane. We choose the vector of magnetic intensity $\vec{A}$ tangent to the loop. We consider the quantum particle with charge $q=-1$ confined to this graph. We set the coefficients $\hbar = 1$, $m = 1/2$. The corresponding Hamiltonian is

$$H\psi = H\begin{pmatrix} g \\ f \end{pmatrix} = \begin{pmatrix} -g'' \\ -f'' - 2\mathrm{i}Af' + A^2 f \end{pmatrix}. \tag{4.30}$$

We consider coupling conditions (4.24) – (4.26) again.

The solution of the Schrödinger equation on the loop is

$$f(x) = C\,\mathrm{e}^{-\mathrm{i}Ax}\sin(kx+\varphi),$$

where C is a constant. We can verify it substituting its derivatives

$$f'(x) = -iCA\,\mathrm{e}^{-\mathrm{i}Ax}\sin(kx+\varphi) + Ck\,\mathrm{e}^{-\mathrm{i}Ax}\cos(kx+\varphi),$$
$$f''(x) = C(-A^2-k^2)\,\mathrm{e}^{-\mathrm{i}Ax}\sin(kx+\varphi) - 2\mathrm{i}CAk\,\mathrm{e}^{-\mathrm{i}Ax}\cos(kx+\varphi)$$

into (4.30).

$$-f''(x) - 2\mathrm{i}Af'(x) + A^2 f(x) = C(A^2+k^2+2\mathrm{i}^2A^2+A^2)\,\mathrm{e}^{-\mathrm{i}Ax}\sin(kx+\varphi)+ \\ + C(2\mathrm{i}Ak - 2\mathrm{i}Ak)\,\mathrm{e}^{-\mathrm{i}Ax}\cos(kx+\varphi) = k^2 f(x). \quad (4.31)$$

From (4.24) we get the condition

$$\sin\varphi = \mathrm{e}^{-\mathrm{i}Al}\sin(kl+\varphi) = \mathrm{e}^{-\mathrm{i}Al}(\sin kl\cos\varphi + \sin\varphi\cos kl),$$
$$\tan\varphi = \frac{\sin kl}{\mathrm{e}^{\mathrm{i}Al} - \cos kl}. \quad (4.32)$$

Before using (4.25) and (4.26) we arrange the term

$$C^{-1}(f'(0) - f'(l)) = -\mathrm{i}A\sin\varphi + k\cos\varphi + \mathrm{i}A\,\mathrm{e}^{-\mathrm{i}Al}\sin(kl+\varphi)- \\ - k\,\mathrm{e}^{-\mathrm{i}Al}\cos(kl+\varphi) = k\left(\cos\varphi - \mathrm{e}^{-\mathrm{i}Al}\cos kl\cos\varphi + \mathrm{e}^{-\mathrm{i}Al}\sin kl\sin\varphi\right) = \\ = k\cos\varphi\,\frac{\mathrm{e}^{\mathrm{i}Al} - \cos kl - \cos kl + \mathrm{e}^{-\mathrm{i}Al}(\cos^2 kl + \sin^2 kl)}{\mathrm{e}^{\mathrm{i}Al} - \cos\varphi} = \\ = k\cos\varphi\,\frac{\mathrm{e}^{\mathrm{i}Al} + \mathrm{e}^{-\mathrm{i}Al} - 2\cos kl}{\mathrm{e}^{\mathrm{i}Al} - \cos kl}. \quad (4.33)$$

We have used the conditions $\sin\varphi = \mathrm{e}^{-\mathrm{i}Al}\sin(kl+\varphi)$ and (4.32).

Now we proceed in the way similar to the example 3. From (4.25) and (4.26) we get

$$f(0) = \alpha^{-1}[f'(0) - f'(l)] + \gamma\,\mathrm{e}^{-3\vartheta/2}g'_\vartheta(0),$$
$$\mathrm{e}^{-\vartheta/2}g_\vartheta(0) = \bar{\gamma}[f'(0) - f'(l)] + \tilde{\alpha}^{-1}\,\mathrm{e}^{-3\vartheta/2}g'_\vartheta(0),$$

substituting $g'_\vartheta(0) = \mathrm{i}k\,\mathrm{e}^{\vartheta}g_\vartheta(0)$ and $f(0) = C\sin\varphi$ we obtain

$$C\sin\varphi = \alpha^{-1}[f'(0) - f'(l)] + \mathrm{i}k\gamma\,\mathrm{e}^{-\vartheta/2}g_\vartheta(0),$$
$$\mathrm{e}^{-\vartheta/2}g_\vartheta(0) = \bar{\gamma}[f'(0) - f'(l)] + \mathrm{i}k\tilde{\alpha}^{-1}\,\mathrm{e}^{-\vartheta/2}g_\vartheta(0).$$

Hence we get the condition

$$(1-\mathrm{i}k\tilde{\alpha}^{-1})\frac{C\sin\varphi-\alpha^{-1}[f'(0)-f'(l)]}{\mathrm{i}k\gamma}=\bar{\gamma}[f'(0)-f'(l)].$$

Using (4.33) we obtain

$$(1-\mathrm{i}k\tilde{\alpha}^{-1})\left[\tan\varphi-\frac{k}{\alpha}\frac{\mathrm{e}^{\mathrm{i}Al}+\mathrm{e}^{-\mathrm{i}Al}-2\cos kl}{\mathrm{e}^{\mathrm{i}Al}-\cos kl}\right]=\mathrm{i}k^2|\gamma|^2\frac{\mathrm{e}^{\mathrm{i}Al}+\mathrm{e}^{-\mathrm{i}Al}-2\cos kl}{\mathrm{e}^{\mathrm{i}Al}-\cos kl}.$$

Now we substitute for $\tan\varphi$ from (4.32) and multiply the equation by $(\mathrm{e}^{\mathrm{i}Al}-\cos kl)/(1-\mathrm{i}k\tilde{\alpha}^{-1})$

$$\sin kl-\left(\frac{k}{\alpha}+\frac{\mathrm{i}k^2|\gamma|^2}{1-\mathrm{i}k\tilde{\alpha}^{-1}}\right)\left(\mathrm{e}^{\mathrm{i}Al}+\mathrm{e}^{-\mathrm{i}Al}-2\cos kl\right)=0.$$

If there is no magnetic field we obtain the condition (4.29). For δ-conditions ($\alpha=\tilde{\alpha}=\gamma^{-1}$) we get the relation

$$-k\frac{\mathrm{e}^{\mathrm{i}Al}+\mathrm{e}^{-\mathrm{i}Al}}{\sin kl}+2k\frac{\cos kl}{\sin kl}+\alpha-\mathrm{i}k=0 \qquad (4.34)$$

From the equations in [5]

$$\left(-k\frac{\mathrm{e}^{\mathrm{i}Al}+\mathrm{e}^{-\mathrm{i}Al}}{\sin kl}+2k\frac{\cos kl}{\sin kl}+\alpha\right)\psi-\mathrm{i}kb=-\mathrm{i}ka, \qquad (4.35)$$

$$\psi=b+a \qquad (4.36)$$

we get for the aplitude of the incoming wave $a=1$ system of two equations for ψ and the amplitude of the outgoing wave b. The denominator of b corresponds to the lhs of (4.34), i. e. the poles of the S-matrix.

Chapter 5

General graph

5.1 Connecting the links

Let us consider a graph with finite many vertices. We suppose that one semiinfinite link is attached to every point from $\mathcal{C} \subset \mathcal{I}$. We denote by f_{jn} the wavefunctions on finite edge of the graph between vertices $\mathcal{X}_j$ and $\mathcal{X}_n$, by g_j the wavefunction on halfline going from vertex $\mathcal{X}_j$.

For every vertex $\mathcal{X}_j \in \mathcal{C}$ which connects a halfline with m lines of the graph

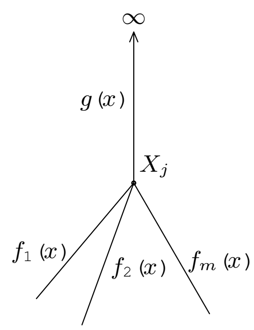

Figure 5.1: Attaching semiinfinite link

we consider coupling conditions

$$f_{j1}(0) = f_{j2}(0) = \ldots = f_{jm}(0) =: f_j(0), \tag{5.1}$$

$$f_j(0) = \alpha_j^{-1} \sum_{n=1}^{m} f'_{jn}(0) + \gamma_j g'_j(0), \tag{5.2}$$

$$g_j(0) = \bar{\gamma}_j \sum_{n=1}^{m} f'_{jn}(0) + \tilde{\alpha}_j^{-1} g'_j(0), \tag{5.3}$$

where function g is wavefunction on the halfline.

For the vertex $\mathcal{X}_j \notin \mathcal{C}$ we assume δ-conditions

$$f_{j1}(0) = f_{j2}(0) = \ldots = f_{jm}(0) =: f_j(0), \tag{5.4}$$

$$\alpha_j f_j(0) = \sum_{n=1}^{m} f'_{jn}(0). \tag{5.5}$$

5.2 Selfadjointness of the Hamiltonian

Let us consider the operator $H = \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)$ with $V_{jn} \in L^\infty([0, l_{jn}])$ and $V_{j\infty} = 0$. Its domain of definition are functions f with components $f_{jn} \in W^{2,2}([0, l_{jn}])$, $f_{j\infty} \in W^{2,2}([0, \infty))$ satisfying the coupling conditions (5.1) – (5.5). Let us denote by H' the same operator only with coupling conditions changed to $f(j) = f'(j) = 0, \forall j \in \mathcal{I}$. This operator has the deficiency indices (n, n). According to the theorem 8.3.1 (c) in [2] are all maximal extensions of this operator selfadjoint. The operator H is an extension of the operator H' and it has the deficiency indices $(0, 0)$.

We verify that the operator H is selfadjoint, i. e. the equality of scalar products $(Hf, \tilde{f}) = (f, H\tilde{f})$ for functions $f, \tilde{f} \in D(H)$. Denoting e the edges of the graph we get

$$\sum_e \int_e \left[\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right) f\right] \bar{\tilde{f}} = \sum_e \int_e f \left[\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right) \bar{\tilde{f}}\right].$$

By integration by parts we obtain for finite edge with length l

$$\int_0^l \left[\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right) f\right] \bar{\tilde{f}} = \int_0^l V f \bar{\tilde{f}} + \int_0^l f' \bar{\tilde{f}}' - \left[f' \bar{\tilde{f}}\right]_0^l =$$

$$= \int_0^l V f \bar{\tilde{f}} - \int_0^l f \bar{\tilde{f}}'' + \left[f \bar{\tilde{f}}' - f' \bar{\tilde{f}}\right]_0^l = \int_0^l f \left[\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right) \bar{\tilde{f}}\right] + \left[f \bar{\tilde{f}}' - f' \bar{\tilde{f}}\right]_0^l.$$

For the edge between vertices $\mathcal{X}_j$ and $\mathcal{X}_n$ (we identify the point $x = 0$ with $\mathcal{X}_j$) we can rewrite the third term

$$\left[f\bar{\tilde{f}}' - f'\bar{\tilde{f}}\right]_0^l = -f(0)\bar{\tilde{f}}'(0) + f'(0)\bar{\tilde{f}}(0) + f(l)\bar{\tilde{f}}'(l) - f'(l)\bar{\tilde{f}}(l) =$$
$$= -f_j\bar{\tilde{f}}'_{jn} + f'_{jn}\bar{\tilde{f}}_j - f_n\bar{\tilde{f}}'_{nj} + f'_{nj}\bar{\tilde{f}}_n.$$

We have denoted by f_j value f at $\mathcal{X}_j$ and by f'_{jn} outward derivative at $\mathcal{X}_j$ (similarly for $\mathcal{X}_n$ and function $\tilde{f}$). That implies the change of signs of last two terms.

The integration over semiinfinite edges is similar, for $f, \bar{\tilde{f}} \in W^{2,2}(0,\infty)$ holds $g(\infty)\bar{\tilde{g}}'(\infty) - g'(\infty)\bar{\tilde{g}}(\infty) = 0$, the redundant term at the point $\mathcal{X}_j$ can be expressed as $g'_j\bar{\tilde{g}}_j - g_j\bar{\tilde{g}}'_j$.

We verify the equality of scalar products

$$\int_\Gamma (Hf)\bar{\tilde{f}} - \int_\Gamma f(H\bar{\tilde{f}}) = 0,$$

that means

$$\frac{1}{2}\sum_{j\in I}\sum_{n\in\nu(j)}(-f_j\bar{\tilde{f}}'_{jn} + f'_{jn}\bar{\tilde{f}}_j - f_n\bar{\tilde{f}}'_{nj} + f'_{nj}\bar{\tilde{f}}_n) + \sum_{j\in I_\mathcal{C}}(g'_j\bar{\tilde{g}}_j - g_j\bar{\tilde{g}}'_j) = 0.$$

Sums $j \in I, n \in \nu(j)$ count every edge of the graph twice, therefore we have to multiply them by $1/2$. Realising that terms $-f_j\bar{\tilde{f}}'_{jn}$ and $f'_{jn}\bar{\tilde{f}}_j$ are in the sum also twice we get simpler condition of selfadjointness

$$\sum_{j\in I}\sum_{n\in\nu(j)}(-f_j\bar{\tilde{f}}'_{jn} + f'_{jn}\bar{\tilde{f}}_j) + \sum_{j\in I_\mathcal{C}}(g'_j\bar{\tilde{g}}_j - g_j\bar{\tilde{g}}'_j) = 0.$$

We split the first sum into sets $I_\mathcal{C}$ and $I\backslash I_\mathcal{C}$

$$\sum_{j\in I_\mathcal{C}}\sum_{n\in\nu(j)}(-f_j\bar{\tilde{f}}'_{jn}+f'_{jn}\bar{\tilde{f}}_j)+\sum_{j\in(I\backslash I_\mathcal{C})}\sum_{n\in\nu(j)}(-f_j\bar{\tilde{f}}'_{jn}+f'_{jn}\bar{\tilde{f}}_j)+\sum_{j\in I_\mathcal{C}}(g'_j\bar{\tilde{g}}_j-g_j\bar{\tilde{g}}'_j) = 0.$$

and use boundary conditions (5.1) – (5.3), (5.4) – (5.5)

$$\sum_{j\in I_C}\sum_{n\in\nu(j)}\left[-\left(\gamma_j g_j' + \alpha_j^{-1}\sum_{k\in\nu(j)} f_{jk}'\right)\bar{\tilde{f}}_{jn}' + f_{jn}'\left(\bar{\gamma}_j\bar{\tilde{g}}_j' + \alpha_j^{-1}\sum_{k\in\nu(j)}\bar{\tilde{f}}_{jk}'\right)\right] +$$
$$+\sum_{j\in(I\setminus I_C)}\sum_{n\in\nu(j)}\left[-\left(\alpha_j^{-1}\sum_{k\in\nu(j)} f_{jk}'\right)\bar{\tilde{f}}_{jn}' + f_{jn}'\left(\alpha_j^{-1}\sum_{k\in\nu(j)}\bar{\tilde{f}}_{jk}'\right)\right] +$$
$$+\sum_{j\in I_C}\left[g_j'\left(\gamma_j\sum_{n\in\nu(j)}\bar{\tilde{f}}_{jn}' + \tilde{\alpha}_j^{-1}\sum_{k\in\nu(j)}\bar{\tilde{g}}_{jk}'\right) - \left(\bar{\gamma}_j\sum_{n\in\nu(j)} f_{jn}' + \tilde{\alpha}_j^{-1}\sum_{k\in\nu(j)} g_{jk}'\right)\bar{\tilde{g}}_j'\right] = 0.$$

After substracting matching terms we obtain

$$\sum_{j\in I_C}\sum_{n\in\nu(j)}(-\gamma_j g_j'\bar{\tilde{f}}_{jn}' + f_{jn}'\bar{\gamma}_j\bar{\tilde{g}}_j') + \sum_{j\in I_C}\sum_{n\in\nu(j)}(\gamma_j g_j'\bar{\tilde{f}}_{jn}' - f_{jn}'\bar{\gamma}_j\bar{\tilde{g}}_j') = 0.$$

5.3 Complex scaling of the semiinfinite links

Now we research how these coupling conditions are changed by scaling the semiinfinite links. We scale the halfline going from the vertex $\mathcal{X}_j$ (for the sake of brevity we drop the subscript j)

$$\begin{aligned}
g_\vartheta(x) &= \mathrm{e}^{\vartheta/2} g(\mathrm{e}^{\vartheta} x),\\
g_\vartheta(0) &= \mathrm{e}^{\vartheta/2} g(0),\\
g_\vartheta'(0) &= \mathrm{e}^{3\vartheta/2} g'(0).\\
g_\vartheta(x) &= \mathrm{e}^{\mathrm{i}k\,\mathrm{e}^{\vartheta} x} g_\vartheta(0), \quad x\in\mathbb{R}^+,\\
g_\vartheta'(x) &= \mathrm{i}k\,\mathrm{e}^{\vartheta} g_\vartheta(0).
\end{aligned}$$

Substituting into (5.1) – (5.3) we get

$$f(0) = \alpha^{-1}\sum_{n=1}^{m} f_n'(0) + \gamma\,\mathrm{e}^{-3\vartheta/2}\mathrm{i}k\,\mathrm{e}^{\vartheta} g_\vartheta(0), \tag{5.6}$$

$$\mathrm{e}^{-\vartheta/2} g_\vartheta(0) = \bar{\gamma}\sum_{n=1}^{m} f_n'(0) + \tilde{\alpha}^{-1}\mathrm{i}k\,\mathrm{e}^{-\vartheta/2} g_\vartheta(0). \tag{5.7}$$

We can easily express $\mathrm{e}^{-\vartheta/2}g_\vartheta(0)$ from (5.7) and substitute it into (5.6).

$$\mathrm{e}^{-\vartheta/2}g_\vartheta(0) = \frac{\bar{\gamma}}{1-\mathrm{i}k\tilde{\alpha}^{-1}}\sum_{n=1}^{m} f_n'(0),$$

$$f(0) = \alpha^{-1}\sum_{n=1}^{m} f_n'(0) + \frac{\mathrm{i}k\gamma\bar{\gamma}}{1-\mathrm{i}k\tilde{\alpha}^{-1}}\sum_{n=1}^{m} f_n'(0).$$

Finally, we obtain

$$f(0) = \left(\alpha^{-1} + \frac{\mathrm{i}k|\gamma|^2}{1-\mathrm{i}k\tilde{\alpha}^{-1}}\right)\sum_{n=1}^{m} f_n'(0).$$

The coefficient in brackets is an effective coupling constant which depends on k, we denote it $\beta(k)^{-1}$. We can express $\beta_j(k)$, where j is index of the corresponding vertex.

$$\beta_j(k) = \frac{\alpha_j}{1+\frac{\mathrm{i}k|\gamma_j|^2\alpha_j}{1-\mathrm{i}k\tilde{\alpha}_j^{-1}}} = \alpha_j\frac{1-\mathrm{i}k\tilde{\alpha}_j^{-1}}{1+\mathrm{i}k(|\gamma_j|^2\alpha_j-\tilde{\alpha}_j^{-1})}. \tag{5.8}$$

The complex coupling constant γ_j controls the connection of the halfline. If $\gamma_j = 0$ then $\beta_j(k) = \alpha_j$.

If the vertex j is not connected with a halfline ($j \notin I_\mathcal{C}$) we have coupling

$$\sum_{n=1}^{m} f_{jn}'(0) = \alpha_j f_j(0), \tag{5.9}$$

otherwise

$$\sum_{n=1}^{m} f_{jn}'(0) = \beta_j(k) f_j(0). \tag{5.10}$$

5.4 The equation for resonances

Now we can proceed in the way similar to the Theorem 3.1 (a) in [4]. We consider the Hamiltonian $H = \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)$ with essentially bounded potential on the internal edges of the graph and no potential on the semiinfinite links. At its vertices we consider δ-coupling with parameter α_j for $j \notin I_\mathcal{C}$ and parameter $\beta_j(k)$ for $j \in I_\mathcal{C}$. We identify the right point of the edge

$\mathcal{L}_{jn} \equiv [0, l_{jn}]$ with the vertex $\mathcal{X}_j$. We denote u_{jn} and v_{jn} solutions of the Schrödinger equation on the edge $\mathcal{L}_{jn}$ which satisfy conditions

$$\begin{array}{rll} u_{jn}(l_{jn}) = 0, & u'_{jn}(l_{jn}) = 1, & \\ v_{jn}(0) = 0, & v'_{jn}(0) = 1 & \text{if} \quad n \in I_{\mathcal{I}}, \\ v_{jn}(0) = \sin\omega_n, & v'_{jn}(0) = -\cos\omega_n & \text{if} \quad n \in I_{\mathcal{B}}, \end{array}$$

where the set $I_{\mathcal{B}}$ and $I_{\mathcal{I}}$ is boundary and interior, respectively, of the graph without semiinfinite links.

The Wronskian of these solutions is

$$W_{jn} = \det \begin{pmatrix} u_{jn}(l_{jn}) & v_{jn}(l_{jn}) \\ u'_{jn}(l_{jn}) & v'_{jn}(l_{jn}) \end{pmatrix} = \det \begin{pmatrix} 0 & v_{jn}(l_{jn}) \\ 1 & v'_{jn}(l_{jn}) \end{pmatrix} = -v_{jn}(l_{jn}),$$

or

$$\begin{array}{ll} W_{jn} = \det \begin{pmatrix} u_{jn}(0) & v_{jn}(0) \\ u'_{jn}(0) & v'_{jn}(0) \end{pmatrix} = \det \begin{pmatrix} u_{jn}(0) & 0 \\ u'_{jn}(0) & 1 \end{pmatrix} = u_{jn}(0) & \text{if} \quad n \in I_{\mathcal{I}}, \\ W_{jn} = \det \begin{pmatrix} u_{jn}(0) & \sin\omega_n \\ u'_{jn}(0) & -\cos\omega_n \end{pmatrix} = -u_{jn}(0)\cos\omega_n - \sin\omega_n u'_{jn}(0) & \text{if} \quad n \in I_{\mathcal{B}}. \end{array}$$

For $n \in I_{\mathcal{I}}$ the transfer matrix on $\mathcal{L}_{jn}$ is

$$T_{nj}(x,0) = W_{jn}^{-1} \begin{pmatrix} u_{jn}(x) - u'_{jn}(0)v_{jn}(x) & u_{jn}(0)v_{jn}(x) \\ u'_{jn}(x) - u'_{jn}(0)v'_{jn}(x) & u_{jn}(0)v'_{jn}(x) \end{pmatrix}.$$

The elements of this matrix can be obtained from the system of the equations

$$\begin{aligned} t_{11}u_{jn}(0) + t_{12}u'_{jn}(0) &= u_{jn}(x), \\ t_{11}v_{jn}(0) + t_{12}v'_{jn}(0) &= v_{jn}(x), \\ t_{21}u_{jn}(0) + t_{22}u'_{jn}(0) &= u'_{jn}(x), \\ t_{21}v_{jn}(0) + t_{22}v'_{jn}(0) &= v'_{jn}(x) \end{aligned}$$

using Cramer's rule.

The transfer matrix between both ends of the edge is

$$T_{nj}(l_{jn},0) = W_{jn}^{-1} \begin{pmatrix} u_{jn}(l_{jn}) - u'_{jn}(0)v_{jn}(l_{jn}) & u_{jn}(0)v_{jn}(l_{jn}) \\ u'_{jn}(l_{jn}) - u'_{jn}(0)v'_{jn}(l_{jn}) & u_{jn}(0)v'_{jn}(l_{jn}) \end{pmatrix} =$$

$$= W_{jn}^{-1} \begin{pmatrix} -u'_{jn}(0)v_{jn}(l_{jn}) & u_{jn}(0)v_{jn}(l_{jn}) \\ 1 - u'_{jn}(0)v'_{jn}(l_{jn}) & u_{jn}(0)v'_{jn}(l_{jn}) \end{pmatrix} = \begin{pmatrix} u'_{jn}(0) & v_{jn}(l_{jn}) \\ \frac{1-u'_{jn}(0)v'_{jn}(l_{jn})}{W_{jn}} & v'_{jn}(l_{jn}) \end{pmatrix}.$$

In the last equality we have used the expressions of the Wronskian.

Denoting $\psi_j := \psi_{jn}(j) \equiv \psi_{jn}(l_{jn})$ and $\psi_n := \psi_{jn}(n) \equiv \psi_{jn}(0)$ we get for the ordinary wave function $\psi_{jn}(x)$

$$\psi_j = u'_{jn}(0)\psi_n + v_{jn}(l_{jn})\psi'_{jn}(n), \tag{5.11}$$

$$-\psi'_{jn}(j) = \frac{1 - u'_{jn}(0)v'_{jn}(l_{jn})}{W_{jn}}\psi_n + v'_{jn}(l_{jn})\psi'_{jn}(n). \tag{5.12}$$

The sign change $\psi'_{jn}(j) = -\psi'_{jn}(l_{jn})$ is because the boundary conditions define the outward derivative.

From (5.11) we get

$$\psi'_{jn}(n) = -\frac{\psi_j - u'_{jn}(0)\psi_n}{W_{jn}},$$

substituting into (5.12) we obtain

$$\psi'_{jn}(j) = -\frac{\psi_n}{W_{jn}} + \frac{v'_{jn}(l_{jn})}{W_{jn}}\psi_j. \tag{5.13}$$

For $n \in I_{\mathcal{B}}$ we get

$$\psi_j = u'_{jn}(0)\psi_n - u_{jn}(0)\psi'_{jn}(n), \tag{5.14}$$

$$-\psi'_{jn}(j) = \frac{u'_{jn}(0)v'_{jn}(l_{jn}) - \cos\omega_n}{W_{jn}}\psi_n + \frac{u_{jn}(0)v'_{jn}(l_{jn}) - \sin\omega_n}{W_{jn}}\psi'_{jn}(n). \tag{5.15}$$

We express

$$\psi'_{jn}(n) = \frac{u'_{jn}(0)\psi_n - \psi_j}{W_{jn}}$$

from (5.14) and substitute into (5.15). We use the relation $\psi_n \cos\omega_n + \psi_j \sin\omega_n = 0$.

$$\psi'_{jn}(j) = \frac{v'_{jn}(l_{jn})}{W_{jn}}\psi_j. \tag{5.16}$$

Now we can substitute the relations (5.13) and (5.16) into (5.9) and (5.10). For $j \notin I_{\mathcal{C}}$ we obtain

$$\sum_{n\in\nu(j)\cap I_I} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{(v_{jn})'(l_{jn})}{W_{jn}} - \alpha_j \right) \psi_j = 0, \tag{5.17}$$

for $j \in I_{\mathcal{C}}$ we get

$$\sum_{n\in\nu(j)\cap I_I} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{(v_{jn})'(l_{jn})}{W_{jn}} - \beta_j(k)\right)\psi_j = 0,$$

Substituting for β_j from (5.8) we obtain the equation for resonances

$$\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{(v_{jn})'(l_{jn})}{W_{jn}} - \alpha_j \frac{1-\mathrm{i}k\tilde{\alpha}_j^{-1}}{1+\mathrm{i}k(|\gamma_j|^2\alpha_j - \tilde{\alpha}_j^{-1})}\right)\psi_j = 0. \tag{5.18}$$

5.5 The S-matrix equation

We find the S-matrix equation in the way similar to the proposition in [5]. The boundary conditions at the point $\mathcal{X}_j \in I_{\mathcal{C}}$ are according to (5.2) and (5.3)

$$\alpha_j\psi_j = \sum_{n\in\nu(j)} \psi'_{jn}(j) + \alpha_j\gamma_j g'_j, \tag{5.19}$$

$$\tilde{\alpha}_j g_j = \tilde{\alpha}_j\bar{\gamma}_j \sum_{n\in\nu(j)} \psi'_{jn}(j) + g'_j. \tag{5.20}$$

The function ψ_{jn} is the wavefunctions on finite link $\mathcal{L}_{jn}$ and $g_j \equiv g_j(0)$ is the value of the wavefunction on the semiinfinite link attached to the point $\mathcal{X}_j$. We can express $g_j(x)$ as a combination of the incoming wave $\mathrm{e}^{-\mathrm{i}kx}$ and the combination of the reflected and the transmited wave $b_j\mathrm{e}^{\mathrm{i}kx}$.

$$g_j(x) = \mathrm{e}^{-\mathrm{i}kx} + b_j\mathrm{e}^{\mathrm{i}kx}. \tag{5.21}$$

For the point $\mathcal{X}_j \notin I_{\mathcal{C}}$ we get from (5.5)

$$\alpha_j\psi_j(j) = \sum_{n\in\nu(j)} \psi'_{jn}(j). \tag{5.22}$$

We can use the equations (5.13) and (5.16) again. Substituting these relations into (5.19) and using the derivative of (5.21) we obtain

$$\alpha_j\psi_j = \sum_{n\in\nu(j)\cap I_{\mathcal{I}}} -\frac{\psi_n}{W_{jn}} + \sum_{n\in\nu(j)} \frac{v'_{jn}(l_{jn})}{W_{jn}}\psi_j + \alpha_j\gamma_j\mathrm{i}k(b_j-1). \tag{5.23}$$

Similarly we get from (5.20)

$$\tilde{\alpha}_j(b_j+1) = \tilde{\alpha}_j\bar{\gamma}_j\left(\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} -\frac{\psi_n}{W_{jn}} + \sum_{n\in\nu(j)} \frac{v'_{jn}(l_{jn})}{W_{jn}}\psi_j\right) + \mathrm{i}k(b_j-1). \quad (5.24)$$

For $j \notin I_{\mathcal{C}}$ we obtain from (5.22)

$$\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{v'_{jn}(l_{jn})}{W_{jn}} - \alpha_j\right)\psi_j = 0. \quad (5.25)$$

Relations (5.23), (5.24) and (5.25) represent a system of $\operatorname{card} I + \operatorname{card} I_{\mathcal{C}}$ equations for variables ψ_j and b_j.

5.6 Comparing both systems of equations

Finally, we compare the condition of solvability of the system of homogenous equations (5.17) and (5.18)

$$\sum_{n\in\nu(j)\cap I_I} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{(v_{jn})'(l_{jn})}{W_{jn}} - \alpha_j\right)\psi_j = 0,$$

$$\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{(v_{jn})'(l_{jn})}{W_{jn}} - \alpha_j\frac{1-\mathrm{i}k\tilde{\alpha}_j^{-1}}{1+\mathrm{i}k(|\gamma_j|^2\alpha_j-\tilde{\alpha}_j^{-1})}\right)\psi_j = 0$$

the condition of unsolvability of the inhomogenous system of equations (5.23), (5.24) and (5.25). If determinant of the system (5.23), (5.24) and (5.25) is zero then b diverges, i. e. we get the condition for poles of the S-matrix.

$$\alpha_j\psi_j = \sum_{n\in\nu(j)\cap I_{\mathcal{I}}} -\frac{\psi_n}{W_{jn}} + \sum_{n\in\nu(j)} \frac{v'_{jn}(l_{jn})}{W_{jn}}\psi_j + \alpha_j\gamma_j\mathrm{i}k(b_j-1),$$

$$\tilde{\alpha}_j(b_j+1) = \tilde{\alpha}_j\bar{\gamma}_j\left(\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} -\frac{\psi_n}{W_{jn}} + \sum_{n\in\nu(j)} \frac{v'_{jn}(l_{jn})}{W_{jn}}\psi_j\right) + \mathrm{i}k(b_j-1),$$

$$\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{v'_{jn}(l_{jn})}{W_{jn}} - \alpha_j\right)\psi_j = 0.$$

From (5.23) we express

$$\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} -\frac{\psi_n}{W_{jn}} + \sum_{n\in\nu(j)} \frac{v'_{jn}(l_{jn})}{W_{jn}}\psi_j = \alpha_j\psi_j - \alpha_j\gamma_j \mathrm{i}k(b_j-1)$$

and substitute it into (5.24)

$$\tilde{\alpha}_j(b_j+1) = \tilde{\alpha}_j\bar{\gamma}_j\left[\alpha_j\psi_j - \alpha_j\gamma_j\mathrm{i}k(b_j-1)\right] + \mathrm{i}k(b_j-1).$$

Hence we obtain

$$b_j - 1 = \frac{\alpha_j\bar{\gamma}_j\psi_j - 2}{1+\mathrm{i}k(\alpha_j|\gamma_j|^2 - \tilde{\alpha}_j^{-1})}$$

and we substitute it into (5.23)

$$\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} \frac{\psi_n}{W_{jn}} - \sum_{n\in\nu(j)} \frac{v'_{jn}(l_{jn})}{W_{jn}}\psi_j - \alpha_j\psi_j + \alpha_j\gamma_j\mathrm{i}k\frac{\alpha_j\bar{\gamma}_j\psi_j - 2}{1+\mathrm{i}k(\alpha_j|\gamma_j|^2 - \tilde{\alpha}_j^{-1})} = 0,$$

$$\sum_{n\in\nu(j)\cap I_{\mathcal{I}}} \frac{\psi_n}{W_{jn}} - \left(\sum_{n\in\nu(j)} \frac{(v_{jn})'(l_{jn})}{W_{jn}} - \alpha_j\frac{1-\mathrm{i}k\tilde{\alpha}_j^{-1}}{1+\mathrm{i}k(|\gamma_j|^2\alpha_j - \tilde{\alpha}_j^{-1})}\right)\psi_j = \\ = \frac{2\mathrm{i}k\alpha_j\gamma_j}{1+\mathrm{i}k(|\gamma_j|^2\alpha_j - \tilde{\alpha}_j^{-1})}. \quad (5.26)$$

We obtain the system of equations (5.25) and (5.26). We can see that the homogenous part of (5.25) and (5.26) gives (5.17) and (5.18). Determinants of both systems of equations are the same, hence the resonance poles obtained by the method of complex scaling are the poles of the S-matrix.

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