A solvable model for scattering on a junction and a modified analytic perturbation procedure.

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The paper is dedicated to Mihail Samoilovich Livshits, who was first to consider a nonselfadjoint operator as a part of an extended selfadjoint scattering system.

Abstract. We consider a one-body spin-less electron spectral problem for a resonance scattering system constructed of a quantum well weakly connected to a noncompact exterior reservoir, where the electron is free. The simplest kind of the resonance scattering system is a quantum network, with the reservoir composed of few disjoint cylindrical quantum wires, and the Schrödinger equation on the network, with the real bounded potential on the wells and constant potential on the wires. We propose a Dirichlet-to-Neumann -based analysis to reveal the resonance nature of conductance across the star-shaped element of the network (a junction), derive an approximate formula for the scattering matrix of the junction, construct a fitted zero-range solvable model of the junction and interpret a phenomenological parameter arising in Datta-Das Sarma boundary condition, see [13], for T-junctions. We also propose using of the fitted zero-range solvable model as the first step in a modified analytic perturbation procedure of calculation of the corresponding scattering matrix.

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AMS subject classification: Primary 47A40, 47A48, 47A55; Secondary 47N50, 47N70, 35Q40.
Key words: Junction, Fitted zero-range model, Dirichlet-to-Neumann map.
1. Introduction

A typical quantum resonance scattering system is composed of a compact inner region surrounded by barriers and an exterior reservoir, where the quantum dynamics is free. These components are weakly connected due to tunneling across the barriers or via a narrow connecting channels. Non-compact quantum networks (QN) are typical resonance scattering systems. Manufacturing of QN with prescribed transport properties is now a most challenging problem of computational nano-electronics. While physical laws defining transport properties of the QN are mostly represented in form of partial differential equations, the direct computing can't help optimization of design of the QN, because it requires expensive and resource consuming scanning over the space of physical and geometrical parameters of the network. The domain of scanning could be essentially reduced in the case when there exist an approximate explicit formula connecting directly the transport characteristics with the parameters defining the geometry and the physical properties of the network.

We derive an explicit approximate formula for the scattering matrix of a simplest QN - a junction, consisting of a vertex domain - a quantum well - connected to the outer reservoir decomposed geometrically into a sum of cylindrical leads. The corresponding model Hamiltonian is obtained based on Glazman splitting, \( L \rightarrow L_\Lambda \oplus l_\Lambda \) of the original Hamiltonian, depending on the Fermi level \( \Lambda \), into the sum of two operators with complementary branches of the continuous spectra. The model proves to be fitted because the corresponding model Dirichlet-to-Neumann map ( DN-map, see [3]) serves a rational approximation of the DN - map of the non-trivial component \( L_\Lambda \) of the split system.

In an important alternative class of the resonance scattering systems, represented by the Helmholtz resonator, the reservoir can’t be decomposed into simple components similar to the cylindrical leads, but the finite leads connecting the compact subsystem - the resonator - with the reservoir, admit a similar decomposition. Then again, a fitted solvable model can be constructed, see [32], based on the splitting of the spectral channels in the leads. The model obtained can serve again as a first step - a jump start - of the corresponding analytic perturbation procedure. We postpone the discussion of the Helmholtz resonator and other systems with nontrivial reservoirs to oncoming publications.

Main difficulty of analysis of resonance scattering systems of both above kinds on the networks is defined by presence of the eigenvalues of the isolated compact subsystem, embedded into the continuous spectrum of the reservoir, separated from the compact subsystem. Indeed, for a selfadjoint operator \( A_0 \) in the Hilbert space \( E \), with discrete spectrum, and small \( \varepsilon V \), the self-adjoint perturbation, \( ||
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\( \varepsilon V \| \leq \varepsilon \), defines, for each simple isolated eigenvalue \( \lambda_0 \) of \( A_0 \)

\[
2\varepsilon < \min_{t \neq s} |\lambda_s - \lambda_t| \equiv \rho_s
\]

a branch of eigenvalues \( \lambda^\varepsilon_s \) of the perturbed operator \( A_\varepsilon := A_0 + \varepsilon V \) represented in form of a geometrically convergent series

\[
\lambda^\varepsilon_s = \lambda_0^s + \varepsilon \lambda_0^s(1) + \varepsilon^2 \lambda_0^s(2) + \varepsilon^3 \lambda_0^s(3) + \ldots,
\]

and the corresponding branch of eigenfunctions, see [28].

This standard analytic perturbation approach is not applicable, generally, to operators with eigenvalues embedded into the continuous spectrum, in particular to non-compact QN where the “spacing” \( \rho \) is zero. Development of radio-location during WWII required analysis of scattering problems on the networks of electromagnetic wave guides, in particular on junctions. The scattering on the junction is a typical perturbation problem for embedded eigenvalues. The perturbation of the problem causes the transformation of real eigenvalues on the vertex domain of the junction into complex resonances. This problem can’t be solved by methods of the standard spectral theory of selfadjoint operators. In the paper [40] M.S. Livshits proposed an elegant approach to the problem of transmission of electro-magnetic signals across the junction, taking into account only oscillatory electro-magnetic modes in the wave-guides and neglecting the “evanescent”- exponentially decreasing modes. He reduced the calculation of the scattering matrix to calculation of the corresponding characteristic function and found a real wave conductance for the oscillatory modes and pure imaginary wave conductance for evanescent modes. The discovery, based on M.S.Livshits ideas, of the connection between the scattering matrix and the characteristic function of the corresponding non-self-adjoint operator, see [1], was an extraordinary achievement and became eventually a source/basement of a series of important results in the theory of the functional models of the dissipative operators, see [39] [50] [49]. The approach to the perturbation theory developed in these papers permitted to understand the spectral nature of the resonances, but it does not help practical problem of optimization of design of quantum or electromagnetic networks with prescribed transport properties. One more detail in the above paper [40] was important in this respect. M.S. Livshits completely disregarded the evanescent waves in the wave-guides, which was usual in the papers of engineers and physicists on the electro-magnetic wave-guides. But he emphasized in [40] importance of accurate elimination of the evanescent waves. This was not done till now. We see now, that the absence of analysis of the evanescent waves prevented M.S. Livshits from establishing, at that time, an effective connection between the geometry of the junction and the transmission/reflection coefficients, see also our comments below, section 3.

In the case of operators with continuous or dense discrete spectrum one can substitute the Hamiltonian \( A_0 \) of an unperturbed system by a fitted solvable model \( A^\varepsilon \), and then develop an analytic perturbation procedure between the perturbed Hamiltonian \( A_\varepsilon \) and the model \( A^\varepsilon \). This two-steps idea \( A_0 \to A^\varepsilon \to A_\varepsilon \) of the modified analytic perturbation procedure was suggested, in implicit form, by H.
Poincare for relevant problems of celestial mechanics, see [62], and formulated in an explicit form in 1972 by I Prigogine. In 1972 I. Prigogine, [63], declared importance of the search of a general practical algorithm for the two-step analytic perturbation procedure

\[ A_0 \rightarrow A^\varepsilon \rightarrow A^\varepsilon \]

implementing the above Poincare idea. Prigogine attempted to find an Intermediate operator \( A^\varepsilon \) as a function of the unperturbed operator \( A^\varepsilon = \Phi(A_0) \), and he wanted to have the above two step analytic perturbation procedure on the whole Hilbert space. The search of the corresponding “intermediate operator” \( A^\varepsilon \) continued for almost 20 years, but did not give any results. Finally Prigogine declared that the intermediate operator with the expected properties does not exist and can’t be constructed.

We guess now, that I Prigogine’s suggestion based on the Intermediate Operator \( A^\varepsilon \) was very close to success. The idea of Prigogine was commonly used by physicists in form of effective Hamiltonian of a complex quantum systems, and, after essential modification, in [38] for “geometrical integration” in dynamical problems of classical mechanics.

In our recent papers [6, 43, 27], see also an extended list of references below, we suggested a method of accurate elimination of the evanescent waves based on the idea of the intermediate Hamiltonian. Our method also permits to accurately eliminate the evanescent waves in the case studied by M.S. Livshits. In this paper we provide, following the quoted papers, a review of the corresponding modified approach to the analytic perturbation procedure and describe, based on [59], an algorithm of construction of the solvable model and the procedure of fitting. We developed the corresponding general approach to the spectral problems with embedded eigenvalues in the series of papers [6, 56, 57, 27, 58, 43, 59, 61]. Contrary to the original Prigogine’s idea, we do a couple of changes:

1. We search for the Intermediate Operator - the “jump start”, see [54] - \( A^\varepsilon \), on the first step of the above mentioned two-step procedure, not among functions \( \Phi(A_0) \) of \( A_0 \), as I. Prigogine suggested, but among weak (finite-dimensional) perturbations of the non-perturbed Hamiltonian \( A_0 \), which is close to the method suggested by Livshits.

2. We restricted our analysis to the part of the unperturbed operator on a spectral subspace which corresponds to some “essential spectral interval”, contrary to I. Prigogine who attempted to find a global Intermediate Operator on the whole space. Thus we develop our modified analytic perturbation procedure locally. A similar requirement of locality is applied in [38] on the space of initial data of the structure-preserving model.

We begin with two classical examples of the resonance scattering systems, to reveal typical difficulties arising from the very beginning when considering perturbations of systems with eigenvalues embedded into the continuous spectrum, and discuss nearest prospects of the perturbative analysis of these systems.

**Example 1: Helmholtz Resonator.**
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Helmholtz resonator was probably the first resonance scattering system discussed mathematically, see [65]. It is composed of the typical details: the inner domain \( \Omega_{\text{int}} \), the shell \( \Omega_{\text{shell}} \), and the reservoir \( \Omega_{\text{out}} \) separated by the shell from \( \Omega_{\text{int}} \).

Consider the Helmholtz equation
\[
-\Delta u = \lambda u \quad \text{in a domain } \Omega \subset \mathbb{R}^3
\]
represented as a sum of two disjoint parts \( \Omega = \Omega_{\text{int}} \cup \Omega_{\text{out}} \) and a shell \( \Omega_{\text{shell}} \) with a small opening.

Kirchhoff suggested to substitute the problem by the model where the opening is pointwise, so that there exist only one common point \( a \in \overline{\Omega_{\text{int}}} \cup \overline{\Omega_{\text{out}}} \cup \overline{\Omega_{\text{shell}}} \).

Kirchhoff suggested an Ansatz for the Green-function \( G_\lambda(x,y) \) of the Helmholtz equation in \( \Omega \) with Neumann boundary condition
\[
-\Delta G_\lambda(x,y) - \lambda G_\lambda(x,y) = \delta(x-y), \quad \frac{\partial G_\lambda}{\partial n} \bigg|_{\partial \Omega} = 0, \quad x, y \in \Omega.
\]
in the form of a linear combination of the Green functions \( G_\lambda^{\text{int}}(x,y) \), \( G_\lambda^{\text{out}}(x,y) \) of the inner and the outer problems:
\[
-\Delta G_\lambda^{\text{in, out}}(x,y) - \lambda G_\lambda^{\text{in, out}}(x,y) = \delta(x-y), \quad \frac{\partial G_\lambda^{\text{in, out}}}{\partial n} \bigg|_{\Omega_{\text{in, out}}} = 0.
\]

![Figure 1. Helmholtz Resonator with a point-wise opening at the point \( a \) and the enlarged detail of the resonator with a narrow short channel, \( \delta \ll H \ll \lambda^{-1/2} \)]

\[
G_\lambda(x,y) = \begin{cases} 
G_\lambda^{\text{out}}(x,y) + A^{\text{out}} G_\lambda^{\text{in}}(x,a), & x, y \in \Omega_{\text{out}} \\
A^{\text{int}} G_\lambda^{\text{in}}(x,a), & y \in \Omega_{\text{out}}, x \in \Omega_{\text{int}},
\end{cases}
\]

with undefined constants -the Kirchhoff coefficients \( A^{\text{out}}, A^{\text{int}} \). This Kirchhoff Ansatz satisfies the equation and the Neumann boundary conditions everywhere.
on \( \partial \Omega \), except the point \( a \), where the Ansatz is singular. The problem of choice of the Kirchhoff constant and other interesting problems concerning the resonator, see \[65\] remained open until recent time, see in this connection the preprint \[10\].

**Example 2: Zero-range potential**

In 1933 E. Fermi, \[18\], considered the problem of scattering of neutrons \( n \) by the nucleon \( S \) of Sulphur. He suggested to choose for this problem the model Hamiltonian in the form of Laplacian in \( L_2(R_3) \) defined on smooth functions \( u \in L_2(R_3) \) with a singularity at the origin

\[
u(x) = \frac{A_u}{4\pi|x|} + B_u + \ldots,
\]

and a special boundary condition imposed on the asymptotic boundary values \( A_u, B_u \):

\[
A_u = \gamma B_u, \quad \gamma = \bar{\gamma}.
\]

The Laplacian is symmetric and even self-adjoint with this boundary condition, and admits explicit calculation of the eigenfunctions: this model is “solvable”. Fermi suggested to “fit” this model choosing \( \gamma = -4\pi p_0^{-1} \), if \( -p_0^2 \) is a small negative eigenvalue in the system \( n, S \).

The model can be extended to the case when \( \gamma > 0 \), and fit to the purely imaginary resonance \( p_0 = i\gamma \). The resulting mysterious “zero-range potential” suggested by Fermi was interpreted by F. Berezin and L. Faddeev \[7\] in terms of von Neumann Operator Extensions Theory, \[47\]. Later this “zero-range potential” was used in numerous physical and mathematical papers and books, see for instance \[4\].

In both above examples the reservoirs are either a large exterior domain, or the whole space with single point \( x = 0 \) removed. The first example was also treated by the operator extension methods in \[17\], producing a zero-range solvable model of the resonator immersed into 3D space. The role of the unperturbed operator in \[17\] played an orthogonal sum of the Neumann Laplacian \( L_{int} \) in \( L_2(\Omega_{int}) \) and \( L_{out} \) in \( L_2(\Omega_{out}) \). The basic difficulty of the original perturbation problem, with a thin short channel, is caused by presence of the eigenvalues of \( L_{int} \) embedded into the continuous spectrum of \( L_{out} \). The standard self-adjoint spectral theory is generally unable to treat the problem of embedded eigenvalues, by observing transformation of them into the corresponding complex resonances. The elegant Lax-Phillips approach to resonance scattering problems reveals the spectral nature or resonances, see \[39\], but does not help to calculate them. In \[17\] the resonances can be easily calculated via solving an algebraic equation, but yet the fitting of the suggested zero-range model remained a problem. In \[10\] an approach to the problem of fitting of the model is suggested based on an explicit formula connecting the “full” scattering matrix of the Helmholtz Resonator with the Neumann-to-Dirichlet map, see \[54\], and a subsequent rational approximation of the Neumann-to-Dirichlet map for the inner domain of the resonator (the cavity \( \Omega_{int} \)). Fortunately the problem of search of the resonances, in the case of small opening, becomes finite-dimensional
after replacement of the Neumann-to-Dirichlet map of the cavity by the corresponding rational approximation, see more details in [10].

In the second example just a self-adjoint operator \(-\Delta_\gamma\) is suggested, with only parameter \(\gamma\), which can be interpreted in spectral terms. This operator plays a role of an effective Hamiltonian of the original scattering problem for the neutrons and the nuclei, see [18]. Yet again, the substitution of the original perturbed (full) Hamiltonian by the effective solvable Hamiltonian \(-\Delta_\gamma\) requires fitting of the model, at least on some essential interval of energy.

Note that the role of the effective Hamiltonian is played, in the second example, by a self-adjoint extension of the unperturbed Hamiltonian \(-\Delta\). Numerous effective Hamiltonians in quantum mechanics are constructed as zero-range solvable models of quantum systems see for instance [53] and our recent papers quoted above.

In this review we represent some results of our recent papers quoted above (see the text preceding the Example 1) where the effective Hamiltonians are constructed as zero-range solvable models. To make the text easily readable, we omit some proofs and most of technical details, which can be found in the original publications. But we pay additional attention to the interconnections of our constructions previously spread in different publications.

2. Scattering on Quantum Networks and Junctions via DN-map.

The basic idea of analysis of partial differential equations on quantum networks is that the corresponding Schrödinger problem can be divided in two parts: a Schrödinger equation on the region surrounded by barriers (e.g. a quantum well) and one on the reservoir the two being weakly coupled by tunneling, see for instance [63] or by a thin channel. It is noticed in [63] that this decomposition “corresponds to the schematization of the transport process as a coherent process on the quantum well, fed by the exterior reservoirs - quantum wires”. On the reservoirs, assumed to be homogeneous and neutral, the electron-electron interaction is neglected, and the single electron is free. But the resonance properties of the quantum well and the tunneling on the contacts define the transport properties of the whole network. It is a common belief that thin quantum network can be modeled by a 1d graph, see [51], with either Kirchhoff boundary conditions, or just non-specified self-adjoint boundary conditions at the vertices. There exist an extended bibliography concerning one-dimensional models of quantum networks, see for instance [12, 36, 37, 25, 72]. Notice that even sharp resonance effects on 2d wave-guides and networks were studied theoretically mainly by numerical methods, see for instance [23, 76].

Quantum network \(\Omega\) which is being studied in this paper, is composed of straight leads (quantum wires) width \(\delta\), some of them semi-infinite, and vertex domains \(\Omega_s\) (quantum wells), see Fig.2. An important basic detail of the quantum network is a junction, see Fig. 3. The junction is a non-compact quantum network com-
Figure 2. Quantum Network: a detail

posed of a quantum well and few semi-infinite quantum wires, of constant width, attached to it. The junction is usually called thin, if the diameter of the quantum well $\Omega_{int}$ strongly dominates the width $\delta$ of the wires $\omega$ attached to it: $\delta << \text{diam } \Omega_{int}$. Calculation of the scattering matrix of a junction is a challenging computational problem, yet accessible for standard commercial programs, see the discussion below. Physicists have certain preferences about the boundary conditions at the vertices, see the discussion below, Example 3.

**Example 3: Thin symmetric T-junction.** For thin symmetric T-junction, with the “bar” orthogonal to the “leg”, a reasonably simple explicit formula for the scattering matrix was suggested in [13] based on reduction of the 2D scattering problem on the junction to the corresponding 1D scattering problem on the corresponding quantum graph, see Fig. 5. The boundary conditions for the model T-junction suggested in [13], is presented in terms of limit values of the wave-function on the 1D wires $\{\psi_i\}_{i=1}^3 := \psi$ and the values of the corresponding outward derivative (boundary currents) $\{\psi'_i\}_{i=1}^3 := \psi'$ at the node:

$$\psi_1 = \beta^{-1} \psi_2 = \psi_3, \quad \psi'_1 + \beta \psi'_2 + \psi'_3 = 0, \quad (1)$$

or in the form

$$P_{\beta}^\perp \tilde{\psi} = 0, \quad P_{\beta} \tilde{\psi}' = 0 \quad (2)$$

with the projection

$$P_{\beta} = \frac{1}{\beta^2 + 2} \begin{pmatrix} 1 & \beta & 1 \\ \beta & \beta^2 & \beta \\ 1 & \beta & 1 \end{pmatrix}. \quad (3)$$
The scattering matrix of such a junction is constant \( S_\beta = I - 2P_\beta \), with the phenomenological parameter \( \beta \) responsible for connection between the bar and the leg. This formula was intensely used, see for instance \([6, 7, 71]\), despite unclear
meaning of the parameter $\beta$. See further discussion of transmission across the junction in [15, 16, 24] and find more references therein.

In this paper, based on the resonance conception of conductance on the junction, we suggest a semi-analytic procedure of calculation of the scattering matrix and a method of reduction of a general thin junction to a quantum graph. Moreover, we suggest a solvable model of a thin junction and reveal the meaning of the projection $P_\beta$. In this paper we do not take into account the spin-orbital interaction, just by disregarding the spin of the electron.

We consider a junction $\Omega$ constructed of a few straight leads $\omega^m$, $\cup_{m=1}^M \omega^m = \omega$, width $\delta$, attached orthogonally to the flat pieces $\Gamma_m$ of the piecewise–smooth boundary of the vertex domain $\Omega_{\text{int}}$, $\Omega = \Omega_{\text{int}} \cup \omega$. On smooth functions $u \in W_2^2(\Omega)$ satisfying the homogeneous Neumann boundary condition, we define the Schrödinger operator

$$- \Delta u + Vu =: \mathcal{L}$$

with the potential $V$ equal to the constant $V_\delta$ on the leads and equal to a real bounded piecewise–continuous function on $\Omega_{\text{int}}$ supplied with Dirichlet boundary condition. The operator $\mathcal{L}$ is essentially self–adjoint, and it can be considered as a perturbation of the corresponding operator $\mathcal{L}_0$ defined by the same differential expression and an additional Dirichlet boundary condition on $\cup_{m=1}^M \Gamma_m = : \Gamma$:

$$\mathcal{L} \rightarrow l^\omega \oplus L_{\text{int}} = \mathcal{L}_0.$$ 

The spectrum $\sigma(L_{\text{int}})$ of $L_{\text{int}}$ is discrete, and the spectrum $\sigma^\omega$ of $L^\omega$ is absolutely continuous, consists of a countable set of branches $\sigma^\omega = \cup_{m=1}^M \cup_{l=1}^\infty \sigma_l^m$ corresponding to the parts $l_l^m$ of $l^\omega$

$$l_l^m = -\frac{d^2}{dx^2} + \frac{\pi^2 l^2}{\delta^2} + V_\delta, \quad l \geq 1,$$

with the homogeneous Dirichlet boundary condition $u|_{\Gamma_m} = 0$ at the bottom sections $x^m|_{\Gamma_m} = 0$. The operators $L_l^m$ on the wires are obtained from $L^\omega$ via separation of
variables, with the basis of cross-section eigenfunctions \(\{e_l^m\} = \left\{\sqrt{\frac{2}{\delta}} \sin \frac{\pi l y}{\delta}\right\}\), \(l = 1, 2, \ldots, m = 1, 2, \ldots M\). Here the local transversal coordinate on \(\omega^m\) is denoted by \(y\). The eigenfunctions of \(L^2\) are scattered waves on each lead \(\omega^m\):

\[
\psi^m_l(x) = \chi^+_l(x) - \chi^-_l(x), \quad x = x_m \geq 0,
\]

represented as linear combinations of oscillating exponential modes

\[
\chi^{m,l}_\pm = e^{\pm i \sqrt{\lambda - \kappa} x} e_l^m(y) := e^{\pm i K^{m,l}_\pm x} e_l^m(y), \quad \lambda > \lambda_l = \pi^2 l^2 \delta^{-2},
\]

with the reflection coefficients \(S_l = 1\). The perturbed operator \(L\) is obtained from \(L_0\) by replacement of the homogeneous Dirichlet boundary condition on the bottom sections \(\Gamma\) by the smooth matching condition. The corresponding scattered waves are obtained via matching on \(\Gamma\) a solution of the Schrödinger equation on the vertex domain with the scattering Ansatz (see for instance \[45, 46\]):

\[
\psi^m_l(x) = \left\{ \begin{array}{ll}
\chi^+_l(x) + \sum_{\pi_2^2/\delta^2 < \lambda} s^{m,m}_{l,r} \chi^+_l(x) + \sum_{\pi_2^2/\delta^2 > \lambda} \xi^{m,m}_{l,r} \chi^+_l(x), & x \in \omega^m \\
\sum_{\pi_2^2/\delta^2 < \lambda} S_l \chi^+_l(x) + \sum_{\pi_2^2/\delta^2 > \lambda} \xi^{m,m}_{l,r} \chi^+_l(x), & x \in \omega^n, \ n \neq m,
\end{array} \right.
\]

composed, for given \(\lambda\), of the above oscillating modes \(\chi^+_l\) in the open channels, with the thresholds below \(\lambda\), \(\lambda^m < \lambda\), and the exponentially decreasing (“evanescent”) modes in the closed channels

\[
\xi^{m,n}_l = e^m_l(y) e^{-i \sqrt{\lambda^m - \kappa} x} := e^{-i K^{m,n}_l x} e^m_l(y), \quad \lambda < \lambda^m,
\]

associated with the thresholds \(\lambda^m = \pi^2 s^2 \delta^{-2}\) of the closed channels in the leads – see \[43\] for details.

The quantum wells and the quantum wires are usually manufactured as a certain relief of the surface of the semiconductor. We assume in this paper that the scaled Fermi level \(\Lambda = 2m*E_F h^{-2}\) of the semiconductor is situated in the middle of the first spectral band \(\Delta_1 = [V_\delta + \frac{4\pi^2}{\delta^2}, V_\delta + 4\pi^2\delta^{-2}]\) of the wire, \(\Lambda = V_\delta + \frac{4\pi^2}{\delta^2}\). Then the first spectral band plays the role of the conductivity band and the junction has metallic properties. At low temperature \(T\), the scattering processes are observed only on the essential spectral interval

\[
\Delta^T = [\Lambda - 2m*\kappa Th^{-2}, \Lambda - 2m*\kappa Th^{-2}] \subset \Delta_1.
\]

If the electron’s density is low, the main contribution to the scattering picture is defined by one-body processes. In this paper we focus on one-body scattering on the essential spectral interval. We disregard the spin-orbital interaction and neglect all effects connected with electrons spin. Hence we study the scattering on the first spectral band \(\Delta_1 = [\pi^2 \delta^{-2}, 4\pi^2 \delta^{-2}]\) of the open channel, and represent the cross-section space \(\mathcal{L}(\Gamma) =: E\) as an orthogonal sum of the entrance subspaces \(E_\pm\) of the open and closed spectral channels respectively:

\[
E_+ = \bigvee_{m=1}^M e^m_l, \quad E_- = \bigvee_{m=1}^M \bigvee_{l=2}^\infty e^m_l, \quad P_{E_{\pm}} =: P_{\pm}.
\]

The infinite linear system for the coefficients of the scattering Ansatz, obtained from the matching conditions, can be solved, if the Green functions \(G_\Gamma^D = G_{int}\)
of the Schrödinger operators $L^D_\Gamma = L_{int}$ in $L_2(\Omega_{int})$, with Dirichlet boundary conditions is constructed. The operator $L^D_\Gamma$ is defined on $W_2^2$-functions in $\Omega_{int}$, with the Meixner conditions at the inner corner points:

$$L_{int}u = -\Delta u + Vu = \lambda u, \ u|_{\partial \Omega_j} = 0. \quad (9)$$

The Green function is found from the equation:

$$L^D_\Gamma G^D_\Gamma = -\Delta G^D_\Gamma + VG^D_\Gamma = \lambda G^D_\Gamma + \delta(x-y), \ G^D_\Gamma|_{\partial \Omega_{int}} = 0. \quad (10)$$

Hereafter we denote by $\sigma^D$ the spectrum of $L^D_\Gamma$. According to the general theory of second–order elliptic equations, the solution $u$ of the boundary problem

$$-\Delta u + Vu = \lambda u, \ u|_\Gamma = u_\Gamma, \ u|_{\partial \Omega_j \setminus \Gamma} = 0. \quad (11)$$

is represented by the Poisson map

$$u(x) = \int_\Gamma \mathcal{P}_\Gamma(x, \gamma, \lambda) u_\Gamma(\gamma) \ d\gamma,$$

involving the kernel $\mathcal{P}_{int}(x, \gamma) = -\partial G^D_\Gamma(x, \gamma)/\partial n_\gamma$. The corresponding boundary current on $\Gamma$ is calculated as

$$\frac{\partial u}{\partial n}|_{x \in \Gamma} = -\int_\Gamma \frac{\partial^2 G^D_\Gamma(x, \gamma, \lambda)}{\partial n_x \partial n_\gamma} u_\Gamma(\gamma) \ d\Gamma =: \mathcal{D}N_\Gamma(\lambda) u_\Gamma.$$

This formal integral operator is restriction onto $\Gamma$ of the Dirichlet-to-Neumann map, see [73, 20, 21]. For the sake of brevity we call it here “relative DN-map”. The relative DN–map is also a Nevanlinna class function $\mathcal{D}N(\lambda)$ for $\text{Im } \lambda \leq 0$, with poles at the eigenvalues of the corresponding Schrödinger operator $L^D_\Gamma = L_{int}$. The relative DN–map is a pseudo–differential operator of order 1: for $W_2^2(\Omega)$ solutions $u$ the DN–map acts from $W^{1/2}(\Gamma)$ to $W^{1/2}(\Gamma)$ and for $W_2^{3/2}(\Omega)$ generalized solutions the D–map acts from $W^{1/2}(\Gamma)$ to $L_2(\Gamma)$.

We consider also the boundary problem

$$-\Delta u + Vu = \lambda u, \ u(\Gamma) = \rho_\Gamma, \ u|_{\partial \Omega_{int} \setminus \Gamma} = 0. \quad (12)$$

and the operator

$$L^N_\Gamma = -\Delta u + Vu, \ u(\Gamma) = 0, \ u|_{\partial \Omega_{int} \setminus \Gamma} = 0. \quad (13)$$

with the relative Neumann Green function $G^N_\Gamma$:

$$L^N_\Gamma G^N_\Gamma = -\Delta G^N_\Gamma + VG^N_\Gamma = \lambda G^N_\Gamma + \delta(x-y), \ G^N_\Gamma|_{\partial \Omega_{int} \setminus \Gamma} = 0, \ \frac{\partial G^N_\Gamma}{\partial n_x}|_{\partial \Omega_{int} \setminus \Gamma} = 0. \quad (14)$$

The map

$$u(x) = \int_\Gamma G^N_\Gamma(x, \gamma, \lambda) \rho_\Gamma(\gamma) d\gamma =: Q^\Gamma_\rho, \ x \in \Omega_{int},$$

involves the kernel $G^N_\Gamma(x, \gamma)$.
A solvable model for scattering on a junction ... gives a solution of the relative Neumann boundary problem (12). The trace of the solution on $\Gamma$
\[ u(x)|_\Gamma = \int_\Gamma G^N_\Gamma(x,\gamma)\rho d\gamma \quad \Gamma = \partial_\psi|_\Gamma = \frac{\partial \psi}{\partial n}|_\Gamma , \quad x \in \Gamma , \]
defines the relative Neumann–to–Dirichlet map which is inverse to the relative Dirichlet–to–Neumann map defined above,
\[ \mathcal{ND}_\Gamma \mathcal{DN}_\Gamma = I \Gamma . \]
For $W^2_2$ solutions $u$ the corresponding DN–map acts, on the set of all regular spectral points $\lambda$ of the Neumann Schrödinger, from $W^{1/2}_2(\Gamma)$ onto $W^{3/2}_2(\Gamma)$. For $W^{3/2}_2$ solutions the ND–map acts acts from $L_2(\Gamma)$ onto $W^{1/2}_2(\Gamma)$. The coefficients of the scattering Ansatz (5) can be found, in principle, from the infinite linear system which is obtained by substitution of the scattering Ansatz into the matching condition (see [43]). An important part of the calculation is the proof of the formula for the DN–map in terms of the $G^D_\Gamma$ (see [43]), or, respectively, a similar formula for the ND–map in terms of $G^N_\Gamma$. Selecting $E_{\pm}$ as indicated above, (8), represent the ND–map of $L^N_\Gamma$ by $2 \times 2$ operator matrix with elements
\[ \mathcal{ND}_{\pm} = P_{\pm} \mathcal{ND}_\Gamma P_{\pm} \]
(15)
The similar decomposition of the DN–map of the Schrödinger operator $L^D_\Gamma$ on $\Omega_{int}$
\[ \mathcal{DN}_\Gamma = \begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix} \]
(16)
was used in [43] in the course of construction of a convenient representation for the scattering matrix on the open spectral bands. We set, in agreement with the above notations in (4,5,6):
\[ K_+ = \sum_m \sum_{open} \sqrt{\lambda - \lambda_1} |e^m_1\rangle \langle e^m| = \sum_m \sqrt{\lambda - \frac{\pi^2}{\delta^2}} |e^m_1\rangle \langle e^m| , \]
\[ K_- = \sum_m \sum_{closed} \sqrt{\lambda - \lambda_1} |e^m_1\rangle \langle e^m| = \sum_m \sum_{l \geq 2} \sqrt{\lambda - \lambda_1} |e^m_1\rangle \langle e^m| . \]
Hereafter we use the standard bra/ket notations, $e << e' : u \rightarrow e << e', u >$, with the bar on the first factor of the dot–product in $E = L_2(\Gamma)$. The exponents of oscillating and decreasing modes on the first spectral band spanned by the vectors $e_{\pm} \in E_{\pm}$ are represented as:
\[ \chi_{\pm} e_{\pm} = e^{\pm iK_{\pm}x} e_{\pm} , \quad \xi_{\pm} e_{\pm} = e^{-K_{\pm}x} e_{\pm} . \]
The matrices $S_{l,r}^{m,n}$ and $s_{l,r}^{m,n}$, which are defined by the matching of the scattering Ansatz to the solution of the homogeneous equation on $\Omega_{int}$, constitute respectively the scattering matrix – the square table of amplitudes in front of the
oscillating modes in open channels \((l = 1)\):

\[
S = \sum_{m,n=1}^{M} \sum_{1,1}^{S_{m,n}} e_{1}^m \langle e_{1}^n \rangle ,
\]

and the table of amplitudes in front of the evanescent modes

\[
s = \sum_{m,n=1}^{M} \sum_{1,2}^{s_{m,n}} e_{1}^m \langle e_{r}^n \rangle .
\]

The scattering matrix of the junction is represented (see [43] and Theorem 2.1 below) in terms of the matrix elements \(DN\), \(NP\) combined in aggregates

\[
M = DN_{++} - DN_{+-} \frac{I}{DN_{--} + K_{-}} DN_{-+}
\]

\[
N = NP_{++} - NP_{+-} K_{-} \frac{I}{NP_{--} + K_{-}} NP_{-+} ,
\]

The width \(\delta\) of the leads can serve as a small parameter in the course of calculation of the scattering matrix. Thin networks, with small \(\delta\), are characterized by large distance between the neighboring spectral thresholds:

\[
\frac{\pi^2 (l + 1)^2}{\delta^2} \frac{\pi^2 l^2}{\delta^2} = (2l + 1) \frac{\pi^2}{\delta^2} .
\]

One can prove following [43] that, for a “thin junction”, the denominator \(DN_{--} + K_{-}\) is invertible on a major part of a properly selected auxiliary spectral interval \(\Delta\), where the DN-map is represented as a sum of a rational function and a regular correcting term:

\[
DN_{\Gamma} = \sum_{\lambda, \in \Delta} \frac{\partial^2 \varphi_{\lambda}}{\partial \varphi_{\lambda}} \frac{\partial \varphi_{\lambda}}{\partial \varphi_{\lambda}} + K_{\Delta} =: DN_{\Delta} + K_{\Delta} ,
\]

The zeros of the denominator \(DN_{--} + K_{-}\) on \(\Delta\) have an important operator-theoretic meaning: they are eigenvalues of the Intermediate Hamiltonian. Hereafter we consider the rational approximation [19] and the corresponding rational approximation of \(DN_{--} = P_{-} DN_{-} P_{-} :\)

\[
DN_{--} = DN_{\Delta} + K_{\Delta} ,
\]

with a regular “error” \(K_{\Delta}\) on a complex neighborhood \(G(\Delta)\) of \(\Delta\).

We call the junction \(\Omega\) thin in closed channels, either in \(W_{2}^{1}(\Gamma)\) or in \(W_{2}^{3/2}(\Gamma)\), if, respectively,

\[
\sup_{\Delta} \| K_{-}^{-1} K_{\Delta}^{-1} \|_{W_{2}^{1}(\Gamma)} < 1 , \quad \text{or} \quad \sup_{\Delta} \| K_{-}^{-1} K_{\Delta}^{-1} \|_{W_{2}^{3/2}(\Gamma)} < 1
\]

This implies the following statement (see [43]):
Lemma 2.1. If the junction is thin on closed channels, then the denominator of (17) is invertible

\[ \left[ \mathcal{K}_-^\Delta + K_- \right]^{-1} : L_2(\Gamma) \to W_2^1(\Gamma), \]

on a corresponding “major part of the essential spectral interval” - the complement of the set of zeros \( Z_\Delta \subset \Delta \) of the determinant of the finite-dimensional matrix-function:

\[ Z_\Delta = \left\{ \lambda : \det \left[ I + (\mathcal{K}_-^\Delta + K_-)^{-1} \mathcal{D} \mathcal{N}_-^\Delta(\lambda) \right] = 0 \} \]

A similar statement holds for the above denominator as an operator from \( W_2^{1/2}(\Gamma) \) to \( W_2^{3/2}(\Gamma) \).

Theorem 2.1. The substitution of the scattering Ansatz (5) into the matching conditions on \( \Gamma \) gives the following formulae for the scattering matrix on \( \hat{\Delta} \)

\[ S = \left[ iK_+ + M \right]^{-1} \left[ iK_- - M \right], \quad (22) \]

\[ S = \left[ NiK_+ + 1 \right]^{-1} \left[ NiK_- - 1 \right]. \quad (23) \]

Proof. The scattering Ansatz generated by the entrance vector \( e \in E_+ \) is constituted by the incoming wave \( e^{iK_+ x} e \), the transmitted/reflected wave \( e^{-iK_+ x} Se \), and the evanescent wave \( e^{-K_- x} se \):

\[ \Psi_e = e^{iK_+ x} e + e^{-iK_+ x} Se + e^{-K_- x} se . \]

The boundary data of the Scattering Ansatz at the bottom sections \( \Gamma \) should match on \( \Gamma \) the boundary data of the solution of the homogeneous Schrödinger equation inside \( \Omega_{int} \):

\[ L_{int} \psi = \lambda \psi, \quad \psi \bigg|_{\partial \Omega_{int} \setminus \Gamma} = 0 , \]

\[ \psi \big|_{\Gamma} = \psi_e(0) = e + Se + se , \quad \frac{\partial \psi}{\partial n} \bigg|_{\Gamma} = \psi'_e(0) = iK_+ e - iK_+ Se - K_- se . \quad (24) \]

Using the matrix representations (16, 15) for \( \mathcal{D} \mathcal{N}, \mathcal{N} \mathcal{D} \), we obtain from (24) two equivalent linear systems which describe matching conditions on \( \Gamma 

\[ iK_+(1 - S)e = \mathcal{D} \mathcal{N}_{++}(1 + S)e + \mathcal{D} \mathcal{N}_{+-} se , \]

\[ -K_- se = \mathcal{D} \mathcal{N}_{-+}(1 + S)e + \mathcal{D} \mathcal{N}_{--} se , \quad (25) \]

and

\[ (I + S)e = \mathcal{N} \mathcal{D}_{++} iK_+(I - S)e - \mathcal{N} \mathcal{D}_{+-} K_- se , \]

\[ [I + \mathcal{N} \mathcal{D}_{--} - K_-] se = \mathcal{N} \mathcal{D}_{-+} iK_+(I - S)e \mathcal{N} \mathcal{D}_{--} se . \quad (26) \]

Eliminating the component \( se \) from them and using the former notations \( M, \mathcal{N} \) we obtain the announced representation for the scattering matrix (22, 23).

The end of the proof

Consider the operator \( \mathcal{L} \) defined by the above Schrödinger differential expression on the junction \( \Omega = \Omega_{int} \cup \omega \), with zero Dirichlet condition on the boundary \( \partial \Omega \).
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It is essentially self–adjoint on the domain of smooth functions $u$, subject to the Meixner restriction $u \in W^1_2(\Omega)$. Assume that the entrance space $E = L^2(\Gamma)$ on the cross–sections $\Gamma$ is decomposed as $E_+ \oplus E_-$. We use the former notations $P_\pm$ for the orthogonal projections in $E$ onto $E_\pm$. Consider the Glazman splitting $\mathcal{L}_\Gamma$ obtained from $\mathcal{L}$ by imposing an additional partial zero boundary condition on the bottom sections $\Gamma$ of the leads:

$$
P_+ u \big|_\Gamma = 0 , \tag{27}$$

complemented by the standard smooth matching condition on $\Gamma$ in closed channels. The operator $\mathcal{L}$ is split by this boundary conditions into an orthogonal sum of two operators:

$$
\mathcal{L} \longrightarrow \mathcal{L}_\Lambda \oplus l_\Lambda = \mathcal{L}_\Lambda .
$$

Here $l_\Lambda = -\frac{d^2}{dx^2} + \pi^2 \delta^2 + V_\delta$ in $L^2(0, \infty) \times E_+ =: \mathcal{H}_+$, with zero boundary condition at the origin $u(0) = 0$, and $L_\Lambda$ is defined in the orthogonal sum of the channel space $L^2(0, \infty) \times E_- =: \mathcal{H}_-$ of the closed channels and $L_2(\Omega_{\text{int}})$ on $W^2_2$ - smooth functions, subject to the Meixner condition and the matching condition on $\Gamma$ in closed channels:

$$
L_\Lambda : D(\Lambda) \longrightarrow L^2(\Omega_{\text{int}}) \oplus \mathcal{H}_-. 
$$

**Theorem 2.2.** The operators $L_\Lambda, l_\Lambda$ are essentially self–adjoint. The absolutely continuous components of spectra of the corresponding self–adjoint extensions are

$$
\sigma_a(l_\Lambda) = [\lambda_1, \infty), \quad \text{with multiplicity } M,
$$

$$
\sigma_a(L_\Lambda) = \bigcup_{l=2}^\infty [\lambda_l, \infty) =: \bigcup_{l \geq 2} \sigma^l_a . \tag{28}
$$

where each branch $\sigma^l_a$ has multiplicity $M$, and the total multiplicity is growing step-wise on the thresholds $\lambda_l$ separating the spectral bands $\Delta_l = [\lambda_l, \lambda_{l+1}]$. The spectral multiplicity of the absolutely–continuous spectrum of $L_\Lambda$ on the spectral bands $\Delta_l$ is equal to $M(l+1)/2$. The discrete spectrum of $L_\Lambda$ consists of a countable set of eigenvalues $\lambda^\Lambda_s$ accumulating at infinity. The singular spectrum of $L_\Lambda$ is empty.

The relation $\mathcal{M} \mathcal{N} = I$ observed from comparison of the formulæ (23, 22) has an important operator–theoretic meaning. It is derived from the fact that $\mathcal{M}, \mathcal{N}$ are respectively DN and ND–maps of the Intermediate Hamiltonian — the part $L^0$ of the Glazman splitting

$$
\mathcal{L} \longrightarrow \mathcal{L}_\Lambda = L_\Lambda \oplus l_\Lambda . \tag{29}
$$

deﬁned by the partial boundary condition $P_+ u \big|_\Gamma = 0$ — see [35]. Contrary to the standard splitting $\mathcal{L} \longrightarrow L_{\text{int}} \oplus L^\omega$, this splitting (29) is ﬁnite–dimensional — see [3]. The poles of $\mathcal{M}$ on the ﬁrst spectral band, below $\lambda_{\text{min}}$, are the eigenvalues of $\Lambda$. 

3. Krein formulae for the intermediate DN-map and ND-map, with the compensated singularities

Expressions $\mathcal{M}, \mathcal{N}$ in the formulae (17, 18) contain, at least formally, the singularities at the eigenvalues of the operators $L^D, L^N$. Presence of these singularities in the conditions of the last theorem of the previous section looks strange. In fact we were able to prove, see [2], that the singularities in the first and second terms of the above Krein formula for $\mathcal{M}$, inherited from $L^D$, compensate each other, so that only the singularities of the denominators of (17) play a role. Similar statement can be proved, see the theorem 3.3 below, for $\mathcal{N}$. But in fact the compensation of singularities permits to obtain more convenient representations for $\mathcal{M}, \mathcal{N}$ - that is for DN and ND maps of the intermediate Hamiltonian $L_\Lambda$. These new representations imply also the corresponding exact formulae for the scattering matrix of $L$, and convenient approximate expressions for the scattering matrix as well. This approximate expressions can serve as base for construction of a fitted solvable model of the junction in form of star-shaped 1D quantum graph, and for derivation of the boundary condition at the vertex.

We begin with the discussion of compensation of singularities in the formula (17) for the DN map $\mathcal{M}$ of the Intermediate Hamiltonian. It appeared, that the singularities of the first and second term at the eigenvalues of $L_{\text{int}}$ compensate each other, so that only the zeros of the denominator $\mathcal{D}_N^- + K^-$ arise as singularities of $\mathcal{D}_N^\Lambda$ on $\Delta$. A one-dimensional version of the statement can be found in [9] and a rescription of the classical Krein formula with compensated singularities is given in [44]. In this paper we review the compensation singularities in Theorem...
following [2] for a general thin junction and prove a similar statement, see Theorem 3.3 for the Intermediate ND-map. We also obtain, in course of calculations, an important “byproduct”: a version of analytic perturbation procedure for groups of eigen-pairs. Note that the standard analytic perturbation procedure is aimed on calculation of an individual perturbed eigenvalue. Usually the convergence of the corresponding perturbation series is limited by the condition of non-intersection of corresponding terms \( \lambda_s(\varepsilon) \neq \lambda_t(\varepsilon) \). Our technique, based on compensation of singularities, can be used even to study overlapping terms and to study the transformation, under small perturbations, of intersections of terms into quasi-intersections. This technique is aimed not on the calculation of an individual perturbed eigenvalue, but rather on derivation of an approximate algebraic equation for the perturbed eigenvalues and calculation of the corresponding residues at the poles of the perturbed DN-map. We also calculate, based on (22), the scattering matrix of a “relatively thin” junction in the quantum network. We also develop similar technique for ND-map. In fact our technique can be modified to calculate the scattering matrix for arbitrary junction, see [2].

For given temperature \( T \) we consider an essential spectral interval centered at the scaled Fermi level \( \Lambda : \Delta_T = [\Lambda - 2m^* T \hbar^{-2}, \Lambda + 2m^* T \hbar^{-2}] \). We assume that the temperature is low, so that \( \Delta_T \) is situated inside the auxiliary spectral interval or an open spectral set \( \Delta \)

\[
\Delta_T \subset \Delta \subset \left( \frac{\pi^2}{\delta^2} + V_\delta, \frac{4\pi^2}{\delta^2} + V_\delta \right) =: \Delta_1.
\]

Our prime aim is: to construct on \( \Delta_T \) a convenient local “quasi-one-dimensional” representation for the intermediate DN-map and one for the scattering matrix \( \Delta \) of the junction with compensated singularities inherited from the \( L_{int} \), to substitute previous formula (22).

Selecting an appropriate spectral interval (or just a spectral set) \( \Delta : \Delta_T \subset \Delta \), we represent the DN-map \( \mathcal{DN} \) of \( L_{int} \) on the essential spectral interval \( \Delta_T \) as a sum

\[
\mathcal{DN}_{int} = \sum_{\lambda_s \in \Delta} \left( \frac{\partial \phi_s}{\partial n} \right) \langle \Gamma \left| \frac{\partial \phi_s}{\partial n} \right| \Gamma \right) + K^\Delta =: \mathcal{DN}^\Delta + K^\Delta.
\]

(30)

of the rational expression constituted by the polar terms with singularities at the eigenvalues \( \lambda_s \in \Delta, s = 1, 2, \ldots N \) of the operator \( L_{int} \) and the analytic operator-function \( K^\Delta \) on a complex neighborhood \( G_{\Delta_T} \) of \( \Delta_T \).

We will also use the operators obtained from \( \mathcal{DN}_{int} \) via framing it by the projections \( P_\pm \), for instance:

\[
P_+ \mathcal{DN}_{int} P_- = P_+ \mathcal{DN}^\Delta P_- + P_+ K^\Delta P_- = \mathcal{DN}^\Delta + K^\Delta.
\]

\[\text{Compare with the popular one-dimensional formula for the scattering matrix in terms of the Weyl function, derived in [52] and intensely used by B. Simon and F. Gezstezy in their approach to the spectral inverse problem, see [19].}\]
We introduce also the linear hull $E^\Delta = \bigvee_{s=1}^N \{ \varphi_s \}$ - an invariant subspace of $L_{int}$, dim $E^\Delta = N$, corresponding to the spectrum of $L_{int}$ contained in $\Delta$ and the part $L^\Delta := \sum_{\lambda_s \in \Delta} \lambda_s \langle \varphi_s \rangle \langle \varphi_s \rangle$ of $L_{int}$ in it. To calculate the intermediate DN-map $\mathcal{M}$ in terms of the standard DN-map of $L_{int}$ we have to solve, see (3.1) the equation:

$$[\mathcal{D}N_{-} + K_{-}]u = \mathcal{D}N_{-} g$$  \hspace{1cm} (31)

on the essential spectral interval $\Delta_T$. It can be solved based on Banach principle if $K_{-}$ can play a role of a large parameter.

**Definition** The junction, for which the operator

$$[K^\Delta_{-} + K_{-}]^{-1}$$  \hspace{1cm} (32)

exists on $\Delta_T$ is called hereafter “relatively thin junction”, for the selected spectral set $\Delta$ and given temperature $T$. A general network is called thin, if all junctions of the network are thin.

For a relatively thin junction, due to continuity of $K^\Delta_{-} + K_{-}$ there exist also a complex neighborhood $G_{\Delta_T}$ of $\Delta_T$, where $K^\Delta_{-} + K_{-}$ is invertible.

Hereafter we assume that the junction is thin. The case of an arbitrary junction is considered in [2].

The above definition of thin junctions (and networks) is based on the following motivation. The DN-map of $L_{int}$ is homogeneous degree $-1$. It acts from $W^{3/2}_{2}(\Gamma)$ to $W^{1/2}_{2}(\Gamma)$, see [73]. If $\Omega_{int}$ has a small diameter $d$ then, the norm of the correcting term $K$ is estimated, generically, on the complement of the spectrum, as Const $1/d$. The same estimate remains true for $P_{-} K^\Delta_{-} P_{-} := K^\Delta_{-}$. The exponent $K_{-}$ on the essential spectral band $\Delta$ acts from $W^{3/2}_{2}(\Gamma)$ to $W^{1/2}_{2}(\Gamma)$ and the norm of its inverse is estimated as Const $\delta$. Then the $W^{3/2}_{2}$-norm of $K^{-1}_{-} K^\Delta_{-}$ is estimated generically as Const $\delta/d$. Hence, in particular, $K_{-} + K^\Delta_{-} = K_{-} [I + K^{-1}_{-} K^\Delta_{-}]$ is invertible if $\delta/d << 1$, see more comments in [43]. Notice, that for arbitrary junction an auxiliary Fermi level $\Lambda^0_F := \Lambda_1$ can be selected, see [2], such that the condition (32) is fulfilled. Now we proceed assuming that (32) is fulfilled.

Consider the part $L^\Delta_{int}$ of $L_{int}$ in the subspace $E^\Delta = \oplus \sum_{\lambda_s \in \Delta} \varphi_s$:

$$L^\Delta_{int} = \sum_{\lambda_s \in \Delta} \lambda_s \varphi_s \langle \varphi_s \rangle : E^\Delta \rightarrow E^\Delta, \text{ dim} E^\Delta = N.$$  

Assume that $\left\{ \frac{\partial \varphi_s}{\partial n} \right\}_{\Gamma}$ are linearly independent. Then $\text{dim} \bigvee_{\lambda_s \in \Delta} \varphi_s = \text{dim} \bigvee_{\lambda_s \in \Delta} \frac{\partial \varphi_s}{\partial n} = N$. Denote by $T$ the map

$$T = \sum_{\lambda_s \in \Delta} \langle \varphi_s \rangle \frac{\partial \varphi_s}{\partial n} \bigg|_{\Gamma},$$  

and introduce

$$\left( P_+ - \frac{I}{K^\Delta_{-} + K_{-}} P_- \right) := \mathcal{J}(\lambda) : E \rightarrow E_+.$$
It is obvious that \( \dim \left\{ \mathcal{J} \frac{\partial \varphi}{\partial n} \right\} \leq \dim E^\Delta \). Later we will utilize a stronger assumption

**Assumption 1** The vectors \( \mathcal{J} \frac{\partial \varphi}{\partial n} \bigg|_\Gamma \) are linearly independent in \( E_+ \) for any \( \lambda \in \Delta \), hence both: \( \dim \left\{ \frac{\partial \varphi}{\partial n} \bigg|_\Gamma \right\} = \dim E^\Delta = N \) and

\[
W_J(\lambda) := \det \left\{ \left( \mathcal{J} \frac{\partial \varphi_s}{\partial n} \bigg|_\Gamma, \mathcal{J} \frac{\partial \varphi_t}{\partial n} \bigg|_\Gamma \right) \right\}_{s,t=1}^N (\lambda) > 0. \tag{33}
\]

The above condition (33) is equivalent to the pair of conditions:

1. The functions \( \frac{\partial \varphi}{\partial n} \bigg|_\Gamma, s = 1, 2, 3 \ldots N \) are linearly independent.

2. The operator \( \mathcal{J}^+ \mathcal{J} \) is invertible in the linear hull \( \bigvee_{s=1}^N \frac{\partial \varphi_s}{\partial n} \bigg|_\Gamma \) for any \( \lambda \in \Delta \).

Hereafter we reduce the problem of compensation of singularities to the spectral analysis of the Schrödinger-type equation

\[
[L^\Delta - Q(\lambda)] \psi = \lambda \psi
\]
in \( E^\Delta \) with the \( \lambda \)-dependent “potential”

\[
Q(\lambda) := T \frac{I}{K^- + K^+} T^+: E^\Delta \to E^\Delta.
\]

**Lemma 3.1.** For thin junction, on the essential spectral interval \( \Delta \) the derivative \( \frac{\partial Q}{\partial \lambda} \) is a positive matrix \( N \times N \).

**Proof.** Recall that the branch of the square root \( \sqrt{\pi^2 \delta^{-2} + V_\delta - \lambda} \) is defined such that \( \frac{dK^\Delta}{d\lambda} < 0 \) on the conductivity band. The correcting term \( K^\Delta \) is a meromorphic operator-function with a negative imaginary part in the upper half-plane \( \mathcal{I} \lambda > 0 \) and a positive imaginary part in the lower half-plane, hence \( \frac{dK^-}{d\lambda} < 0 \) on the conductivity band \( \Delta_1 \). This implies:

\[
\frac{\partial Q}{\partial \lambda} = -T \frac{I}{K^- + K^+} \left[ \frac{dK^-}{d\lambda} + \frac{dK_+^\Delta}{d\lambda} \right] \frac{I}{K_-^\Delta + K^-} T^+ > 0, \quad \text{for} \ \lambda \in \Delta_T \in \Delta_1.
\]

The end of the proof

Based on some cumbersome calculation, we are able to derive, see [2], that all singularities in the Krein formula, inherited from the eigenvalues \( \lambda_s \) of the unperturbed operator \( L_{int} \), are compensated.

**Theorem 3.1 (Compensation of Singularities M.).** The Krein formula \( [T^+ \mathcal{J}] \) for the intermediate DN-map, can be re-written, for a thin junction, on the spectral interval \( \Delta \), as:

\[
\mathcal{M} = D^\Delta N^\Delta = \mathcal{M}_{\text{reg}} + [T^+ \mathcal{J}] \left( I_{\mathcal{M}^\Delta - L^\Delta + Q(\lambda)} [T^+ \mathcal{J}].
\]

A solvable model for scattering on a junction . . .

\[ k(\lambda) + J^T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q(\lambda)}(TJ^+, \lambda) =: k(\lambda) \]

where \( K^\Delta_{\pm} - K^\Delta_{\pm} =: k(\lambda) \) is a regular part of \( M \) on \( \Delta_T \). The representation (34) remains valid on a complex neighborhood \( G_{\Delta} \) of the spectral interval \( \Delta \).

**Remark 1** The announced rescription (34) of the Krein formula (17) for the DN-map of the intermediate Hamiltonian, has on the essential spectral interval only non-compensated singularities, at the eigenvalues of the intermediate Hamiltonian, calculated as zeros \( \lambda_Q^s \) of the denominator \( \lambda I^\Delta - L^\Delta + Q(\lambda) := d(\lambda) \) :

\[ d(\lambda_Q^s) \nu_Q^s = 0. \]

These singularities coincide with the eigenvalues of the intermediate Hamiltonian. We call the above formula (34) for \( \Lambda \) the modified Krein formula. Inserting (34) into the above formula (22) gives a convenient representation for the scattering matrix of the relatively thin junction, which permits, in particular, to calculate sharp resonances, situated near the continuous spectrum, based on eigenvalues of the intermediate operator.

In the case of one-dimensional zeros of the denominator \( d(\lambda_Q^s) \nu_Q^s \neq 0 \), the corresponding residues are calculated as projections onto the subspaces

\[ E_Q^s = J(\lambda_Q^s)T^+ \nu_Q^s. \]

For multidimensional zeros of the denominator, \( d(\lambda_Q^s)N_Q^s = 0 \), \( \dim N_Q^s > 1 \) the residues are projections onto the images of the corresponding null-spaces \( N_Q^s = \bigvee_s \nu_Q^s \)

\[ E_Q^s = J(\lambda_Q^s)T^+ N_Q^s. \]

The above expression (34) is analytic in \( \Omega_{\Delta} \) on the complement of the set of zeros of the denominator \( d(\lambda) \). This means that the eigenvalues of the Intermediate Hamiltonian are selected from the set. Assume that \( \lambda_Q^s, s = 1, 2, 3, \ldots N \) are simple zeros of the denominator.

**Theorem 3.2.** If the Wronskian (33) does not vanish at the algebraically simple (first order) zero \( \lambda_Q^1 \) of the denominator, \( W_J(\lambda_Q^1) \neq 0 \), then the zero is an eigenvalue of the Intermediate Hamiltonian, with the same spectral multiplicity.

**Proof.** It is sufficient to prove, that the zero is a first order pole of the intermediate DN-map, with a finite-dimensional residue having the same dimension as the zero of the denominator. Consider the equation

\[ d(\lambda)u = [\lambda I^\Delta - L^\Delta + Q(\lambda)] \]

Assume that \( d(\lambda_Q^1)\nu_Q^1 = 0 \), and denote by \( P_Q^1 \) an orthogonal projection onto the multiple eigen-space \( \bigvee_s \nu_Q^s \) of the operator \( L^\Delta - Q(\lambda_Q^1) =: L_Q^1 \), and by \( R_Q^1 \) the corresponding resolvent:

\[ \left[ L^\Delta - Q(\lambda_Q^1) - \lambda I^\Delta \right]^{-1} = R_Q^1(\lambda). \]
Then, for $\lambda$ close to $\lambda_Q^1$ we can substitute the “potential” $Q$ in the above equation by the Taylor expansion:

$$Q(\lambda) = Q(\lambda_Q^1) + (\lambda - \lambda_Q^1) \frac{dQ}{d\lambda}(\lambda_Q^1) + \frac{(\lambda - \lambda_Q^1)^2}{2} \frac{d^2Q}{d\lambda^2}(\lambda_Q^1) + \ldots$$

and represent the resolvent near the pole $\lambda_Q^1$ as

$$R^Q_\chi = \frac{P_1}{(\lambda_Q^1 - \lambda)} + R^Q_{\perp, \lambda_Q^1},$$

where $R^Q_{\perp, \lambda_Q^1}$ is the part of the resolvent in the complementary invariant subspace $E^1_\perp = (I - P_1)E$. Replacing $Q(\lambda)$ by the corresponding first order Taylor formula, we rewrite the equation $d(\lambda)u = f$ by the equation

$$u + R^Q_\chi (\lambda_Q^1 - \lambda) \frac{dQ}{d\lambda} u = -R^Q_\chi f. \quad (37)$$

To calculate the residue of the solution $u$ at the pole $\lambda_Q^1$ we multiply (37) by $\frac{dQ}{d\lambda}$ and by the spectral projection $P_1^Q$ of $L_\Delta^Q$ at $\lambda_Q^1$ and take into account that the resolvent $R^Q_\chi$ of $L_\Delta^Q$ has a simple pole and neglect the terms vanishing at $\lambda_Q^1$, in particular all terms arising from the above Taylor expansion beginning from the second $(\lambda - \lambda_Q^1)^2 \frac{d^2Q}{d\lambda^2}(\lambda_Q^1)$. Due to positivity of $\frac{dQ}{d\lambda}$ the operator $I + P_1^Q \frac{dQ}{d\lambda} P_1^Q$ is invertible. Then, due to (36)

$$P_1^Q \frac{dQ}{d\lambda} u = \frac{I}{I + P_1^Q \frac{dQ}{d\lambda} P_1^Q} P_1^Q \frac{dQ}{d\lambda} R^Q_\chi f$$

has the polar part at $\lambda_Q^1$

$$u = -\frac{P_1^Q \left[ I + P_1^Q \frac{dQ}{d\lambda} P_1^Q \right]^{-1} P_1^Q}{\lambda_Q^1 - \lambda} f + \ldots \quad (38)$$

The operator in the square bracket is positive and hence has the spectral form:

$$P_1^Q \left[ I + P_1^Q \frac{dQ}{d\lambda} P_1^Q \right]^{-1} P_1^Q = \sum_r \alpha_r \langle \nu_r | \nu_r \rangle.$$

Then the polar term of $d^{-1}$ is $-\left[ L_\Delta^Q(\lambda) \right]^{-1}$ at $\lambda_Q^1$ is $(\lambda - \lambda_Q^1)^{-1} \sum_r \alpha_r \langle \nu_r | \nu_r \rangle$ and the pole part of the intermediate DN-map at $\lambda_Q^1$ is

$$DN^\Lambda_{\text{pole}} = \sum_r \lambda \langle JT^+ \nu_r | \nu_r \rangle \alpha_r \langle JT^+ \nu_r | \nu_r \rangle \lambda - \lambda_Q^1.$$

Due to the orthogonality of $\nu_r$ and non-degeneracy of the Wronskian $W^Q_{\Delta}$, the vectors $JT^+ \nu_r$ are linearly independent, hence $\lambda_Q^1$ is a simple pole of the intermediate DN-map, with the spectral multiplicity $\dim \bigwedge \nu \in_c Q$.

The end of the proof.
A solvable model for scattering on a junction . . . 23

The scattering matrix of the original problem on the essential spectral interval can be obtained via replacement in (22) the intermediate DN-map by the expression (34) with compensated singularities. This substitution is possible for thin junctions, when the exponent $K_-$ in closed channels can play a role of a large parameter, compared with the error $K_\Delta - K_\Delta^\Delta$ of the rational approximation $DN_\Delta$ of $DN$.

This condition may be not satisfied, for given quantum network, at the scaled Fermi level $\Lambda$. In that case another representation of the scattering matrix (23) can help.

We consider now the problem of compensation singularities for the intermediate ND-map $N$ on the essential spectral interval.

Denote by $\psi_s, \lambda_s^N$ the eigen-pairs of the operator $L_\Gamma$, see (13). Select the eigen-values from the spectral interval $\Delta_2$, to be defined later, and introduce $E_{1\Delta_2}^N := \bigvee_{\lambda_s^N \in \Delta_2} \psi_s$ and $E_{2\Delta_2}^N := \bigvee_{\lambda_s^N \in \Delta_2} \psi_s|_{\Gamma}$, and consider the map

$$\tilde{T} : \sum_{\lambda_s^N \in \Delta_2} \psi_s|_{\Gamma} \langle \psi_s : E_{\Delta_2} \to E_{1\Delta_2}^N, s = 1, 2, \ldots \hat{N}$$  (39)

**Assumption 2**, see the paragraphs 1 and 2 below:

1. We assume that the families $\{\psi_s\}_{s=1}^N$, $\{\psi_s\}_{s=1}^N|_{\Gamma}$ are linearly independent, thus are bases in their linear hulls $E_{1\Delta_2}^N$, $E_{2\Delta_2}^N$, $\dim E_{1\Delta_2}^N = \dim E_{2\Delta_2}^N = \hat{N}$.

Represent the compact in $L_2(\Gamma)$ relative ND-map $ND_{1\Gamma} := ND^F$ as

$$ND_{1\Gamma} = \begin{pmatrix} ND_{++} & ND_{+-} \\ ND_{-+} & ND_{--} \end{pmatrix} = \sum_{\lambda_s^N \in \Delta_2} \frac{\psi_s|_{\Gamma}}{\lambda_s^N - \lambda} \langle \psi_s |_{\Gamma} + \hat{\kappa}_{\Delta_2}^2 =: ND_{1\Delta_2}^2 + \hat{\kappa}_{\Delta_2}$$

and consider the corresponding matrices

$$ND_{1\Delta_2}^2 = \begin{pmatrix} ND_{++} & ND_{+-}^2 \\ ND_{-+}^2 & ND_{--}^2 \end{pmatrix},$$

and

$$\hat{\kappa}_{\Delta_2} = \begin{pmatrix} \hat{\kappa}_{+} & \hat{\kappa}_{+}^2 \\ \hat{\kappa}_{-}^2 & \hat{\kappa}_{-} \end{pmatrix} =: \hat{\kappa},$$

in the basis $E_+, E_-$ of $E = L_2(\Gamma)$. Hereafter we omit the upper index $\Delta_2$ on matrix elements $\hat{\kappa}_{\pm \pm}$. To represent $ND_{1\Gamma} := N$ in the form with already compensated singularities inherited from the resolvent of $L_\Gamma$, we have to solve the equation

$$(I + ND_{--}) u = ND_{++} f$$  (40)

Our second basic assumption is the following:

2. We assume, that the width $\delta$ of the leads, the essential spectral interval $\Delta_T := \Delta \subset \Delta_2$ and the rational approximation $\hat{\kappa}$ are selected such that

$$I + \hat{\kappa}_{\Delta_2}^2 K_-$$  (41)

is invertible for $\lambda \in \Delta$. 


For low temperature (that is for a relatively small essential spectral interval $\Delta_T$) this condition is equivalent to the corresponding condition imposed just at the scaled Fermi level $\Lambda$. It is satisfied, if

$$\sup_{\lambda \in \Delta} \| \hat{\mathcal{K}}_{\lambda} - K_{\lambda} \| < 1. \quad (42)$$

We will not give here a formal condition which guarantees 2, but just notice that due to compactness of the resolvent on $L^2$ for any $\Delta_T$ there exist $\Delta_2 \supset \Delta_T$ and the corresponding number $\hat{N}_{\Delta_2} =: \hat{N}$ such that the error of the finite rational approximation of the resolvent is small:

$$G^N(x, s, \lambda) = G^N(x, s, \mu) + (\lambda - \mu)Q^\Delta_2 =$$

$$G^N(x, s, \mu) + (\lambda - \mu)\sum_{i=1}^{\hat{N}} \frac{\varphi_i(x)}{(\lambda_i - \mu)^2} + (\lambda - \mu)^2 \sum_{i=N+1}^{\infty} \frac{\varphi_i(x)}{(\lambda - \lambda_i)(\lambda_i - \mu)^2} =$$

$$G^N(x, s, \mu) + \hat{Q}_2(x, s, \lambda, \mu) + \hat{\mathcal{K}}^\Delta_2(x, s, \lambda, \mu) =: \hat{Q}(x, s, \lambda, \mu) + \hat{\mathcal{K}}(x, s, \lambda, \mu). \quad (43)$$

Here we choose $\mu$ large negative, so that $G^N(x, s, \mu)$ is a kernel of a small integral operator and denote hereafter

$$G^N(x, s, \mu) + \hat{\mathcal{K}}^\Delta_2(x, s, \lambda, \mu) =: \hat{\mathcal{K}}(x, s, \lambda, \mu), \quad \hat{Q}_2(x, s, \lambda, \mu) = \hat{N}\mathcal{D}(x, s, \lambda, \mu).$$

Then for the error $P_-\hat{\mathcal{K}}P_- =: \hat{\mathcal{K}}_-$ of the rational approximation $\hat{Q}$ framed by the projections onto $E_-$ the corresponding estimate (12) is valid. Denote

$$\hat{\mathcal{K}}_{++} - \hat{\mathcal{K}}_{+-} K_- (I + \hat{\mathcal{K}}_{--} K_-)^{-1} \hat{\mathcal{K}}_{-+} =: \hat{N}_{reg},$$

$$\left\{ P_+ - \hat{\mathcal{K}}_{+-} K_- (I + \hat{\mathcal{K}}_{--} K_-)^{-1} \right\} \hat{T}^+ =: \hat{\mathcal{T}} \hat{T}^+,$$

$$\hat{T} K_-(I + \hat{\mathcal{K}}_{--} K_-)^{-1} \hat{T}^+ =: V(\lambda)$$

$$L^\Delta = \lambda L^\Delta + V(\lambda) =: L^\Delta(\lambda),$$

$$\hat{T} \left\{ P_+ - K_-(I + \hat{\mathcal{K}}_{--} K_-)^{-1} \hat{\mathcal{K}}_{--} \right\} =: \hat{T} \hat{\mathcal{T}}^+. \quad (44)$$

**Theorem 3.3. (Compensation of Singularities N)**

$$\mathcal{N} = \mathcal{N}_{reg} - \hat{\mathcal{T}} \hat{T}^+ \frac{1}{L^\Delta(\lambda)} \hat{T} \hat{\mathcal{T}}^+ \quad (45)$$

**Proof** We treat the equation (40) with use of the Banach principle under assumption (42):

$$K_- u + K_-(I + \hat{\mathcal{K}}_{--} K_-)^{-1} \mathcal{N}^\Delta \hat{K}_- u = K_-(I + \hat{\mathcal{K}}_{--} K_-)^{-1} \mathcal{N}^\Delta f. \quad (46)$$

Recall that $\mathcal{N}^\Delta = \mathcal{N}^\Delta \hat{K} + \hat{K}$ and notice that $\mathcal{N}^\Delta \hat{K}$ is connected with the part $L^\Delta$ of $L^N$ in $E^\Delta$ as

$$\mathcal{N}^\Delta = \hat{T}^+ \frac{1}{L^\Delta(\lambda)} \hat{T}.$$

Then, denoting

$$\frac{1}{L^\Delta - \lambda I^\Delta} \hat{T} K_- u =: v$$
The terms which do not contain singularities result in:

\[ v = [L^{A_2}(\lambda)]^{-1} V \frac{I}{L^{A_2} - \lambda I^{A_2}} \tilde{T} P_+ f. \]

Substituting the result into (46)

\[ K_- u = K_- (I + \tilde{K}_- K_-)^{-1} \left\{ \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} \tilde{T} + \tilde{K}_- \right\} P_+ f - \tilde{T} [L^{A_2}(\lambda)]^{-1} \tilde{T} K_- (I + \tilde{K}_- K_-)^{-1} \left[ \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} \tilde{T} + \tilde{K}_- \right] P_+ f. \]

Then \( N f \) =

\[ P_+ \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} \tilde{T} P_+ f + \tilde{K}_- f - P_+ \left[ \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} \tilde{T} P_- + \tilde{K}_- \right] \times \]

\[ K_- (I + \tilde{K}_- K_-)^{-1} \left\{ \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} \tilde{T} + \tilde{K}_- \right\} P_+ f - \tilde{T} [L^{A_2}(\lambda)]^{-1} \tilde{T} K_- (I + \tilde{K}_- K_-)^{-1} \left[ \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} \tilde{T} + \tilde{K}_- \right] P_+ f \right\}. \]

Leading terms inside parentheses give:

\[ K_- (I + \tilde{K}_- K_-)^{-1} \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} V \frac{I}{L^{A_2} - \lambda I^{A_2}} = \]

\[ K_- (I + \tilde{K}_- K_-)^{-1} \tilde{T} + \frac{I}{L^{A_2}(\lambda)}. \] (47)

Taking into account the leading term of the first addendum, we obtain:

\[ P_+ \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} \tilde{T} P_+ f - \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} V \frac{I}{L^{A_2}(\lambda)} \tilde{T} P_+ f = \]

\[ P_+ \tilde{T} + \frac{I}{L^{A_2}(\lambda)} \tilde{T} P_+ f. \] (48)

Lower order terms containing \( \frac{I}{L^{A_2} - \lambda I^{A_2}} \) in parentheses give:

\[ -\tilde{K}_+ K_- (I + \tilde{K}_- K_-)^{-1} \tilde{T} + \frac{I}{L^{A_2} - \lambda I^{A_2}} V \tilde{T} f = \]

\[ -\tilde{K}_+ K_- (I + \tilde{K}_- K_-)^{-1} \tilde{T} + \frac{I}{L^{A_2}(\lambda)} \tilde{T} P_+ f, \] (49)

and the adjoint expression. The term which contains only the main singularity \([L^{A_2}(\lambda)]^{-1}\) is

\[ \tilde{K}_+ K_- (I + \tilde{K}_- K_-)^{-1} \tilde{T} + \frac{I}{L^{A_2}(\lambda)} \tilde{T} K_- (I + \tilde{K}_- K_-)^{-1} \tilde{K}_+ \]

The terms which do not contain singularities result in:

\[ \tilde{K}_{++} - \tilde{K}_{++} K_- (I + \tilde{K}_- K_-)^{-1} \tilde{K}_{++} =: N_{reg} \] (50)
Note that the operator $K_-(I + \tilde{K}_-K_-)^{-1}$ is self-adjoint on the first spectral band. Then, collecting all terms we obtain the announced result.

The end of the proof

Based on the theorems 3.1, 3.3 we can calculate the scattering matrix either in the form (22) or in the form (23). One of these formulae can be more convenient on the essential spectral interval, than another, depending on localization of singularities of $DN$ and $ND$. Luckily, due to $DN = ND = I_+$, the singularities of the factors do not overlap, hence for any point $\lambda_0 \in \Delta$ one can select an interval centered at $\lambda_0$ where at least one of the factors $DN$ or $ND$ can be substituted by the corresponding approximate expression based on the bi-linear formulae suggested in [60].

4. Approximate Scattering Matrix and the boundary condition at the vertex of the quantum graph

The standard method of calculation of the scattering matrix requires solving of an infinite algebraic system anyway, though practically admits a certain simplification in closed channels, see [45], where it was done for waveguides with simple geometry. The approach based on the intermediate DN-map gives a finite linear system for the scattering matrix derived from matching of the component $\Psi_+$ of the scattering Ansatz on the first (open) channel in wires with $p = \sqrt{\lambda - V_\delta - \pi^2 \delta^2}$, on the first spectral band $\Delta_1$:

$$\Psi_+ e_+ := e^{ip\xi}e_+ + e^{-ip\xi}S(p)e_+$$

(51)

to the limit values on the spectrum, $\Im \lambda \to 0$, of the solution of an intermediate boundary problem with the boundary data on $\Gamma$ defined by the scattering Ansatz $\Psi$. The boundary data $\Psi|_\Gamma$, $\frac{\partial \Psi}{\partial n}|_\Gamma$ are connected by the intermediate DN-map, hence the required matching gives a finite linear system for $S$:

$$ip [e_+ - S(p)e_+] = M(\lambda) [e_+ + S(p)e_+] .$$

(52)

Solving this equation we obtain the formula for the scattering matrix of the operator $L$ on the first spectral band $\Delta_1$ in terms of $L_\Lambda$ by the formula, see (22).

Due to Theorem 3.2 one can substitute, for a thin junction, the intermediate DN-map $M(\lambda)$ in (22) by an approximate expression for $M = M_\Delta + K_\Delta$, where $M_\Delta := M_{\text{approx}}$ is a rational approximation $DN$ of $M$ on the essential spectral interval $\Delta_T$, containing only polar terms with poles on an auxiliary spectral interval $\Delta$, and $K_\Delta$ is a regular part of $M$ on $\Delta$.

**Theorem 4.1.** The resulting approximate expression for the scattering matrix

$$S \approx [ipP_+ + M_\Delta]^{-1}[ipP_- - M_\Delta] =: S_{\text{approx}},$$

(53)

with $p = \sqrt{\lambda - V_\delta - \pi^2 \delta^2}$, can be used as a first step for the calculation of the exact scattering matrix via an analytic perturbation procedure.

\footnote{The author is grateful to V. Katsnelson for important comments in that connection.}
Proof  Indeed, due to the above theorem \[3.2\] the error \[M - M_{\text{approx}} = \mathcal{K}^\Delta,\] with \[\mathcal{K}^\Delta\] containing the regular term \[M_{\text{reg}}\] too, is real and estimated by \[O(\delta d_{\text{int}}^{-2}).\] Then, due to \[3.1\] we can represent the exact scattering matrix in form of a product:

\[
S = \left( I + [ipP_+ + M^\Delta]^{-1}K^\Delta \right)^{-1} S_{\text{approx}} \left( I - [ipP_+ - M^\Delta]^{-1}K^\Delta \right). \tag{54}
\]

Here \[M^\Delta, K^\Delta\] are hermitian on \[\Delta_1\], hence \[\| [ipP_+ \pm M^\Delta]^{-1} \| << \delta, \] for thin junctions. Hence the analytic perturbation procedure of the calculation the left and right factors of the expression in \(54\) is geometrically convergent due to \(\delta O(\delta d_{\text{int}}^{-2}) << 1.\) Thus the exact scattering matrix can be obtained from \[S_{\text{approx}}\] by an analytic perturbation procedure.

The end of the proof

One can construct various approximations for the scattering matrix based on \[S_{\text{approx}},\] replacing \[M\] by various approximate expressions, with controllable errors, see for instance \[58,59\].

\section{Simple resonance eigenvalue of the Intermediate Hamiltonian}

The simplest approximate formula for the scattering matrix can be obtained in the case when there exist a single simple eigenvalue \[\lambda_1^\Lambda\] of the Intermediate Hamiltonian on the auxiliary spectral interval \[\Delta\]. Indeed, substituting the intermediate DN-map \[M = \mathcal{K}^\Lambda + \alpha_1^\Lambda \frac{P_\perp}{\lambda - \Lambda} \] by the corresponding polar approximation generated by the resonance eigenvalue \[\lambda_1^\Lambda\] of the Intermediate Hamiltonian and the boundary current of the corresponding eigenfunction

\[
\alpha_1^\Lambda P_1^\Lambda = P_+ \frac{\partial \varphi^\Lambda}{\partial n} \mid_\Gamma \) \langle P_+ \frac{\partial \varphi^\Lambda}{\partial n} \mid_\Gamma =: \psi_1^\Lambda \rangle \langle \psi_1^\Lambda,
\]

we are able to obtain, due to preceding theorem \(4.1\), the scattering matrix of a thin junction via an analytic perturbation procedure based on the jump-start

\[
S_{\text{jump-start}} = \left[ ik_+ + k(\lambda) + \alpha_1^2 \frac{P_1^\Lambda}{\lambda - \Lambda} \right]^{-1} \left[ ik_+ - k(\lambda) - \alpha_1^2 \frac{P_1^\Lambda}{\lambda - \Lambda} \right]. \tag{55}
\]

In the case when the first spectral band \[\Delta_1\] is the conductivity band \(\Lambda\), the above approximate expression for the scattering matrix can be represented, with \[P_\perp = P_+ \ominus P_1^\Lambda\] and \[p_1 = \sqrt{\lambda - \pi^2 \delta^2 - \nu_0^2}\] and \[\lambda_1^\Lambda \approx \Lambda\] as:

\[
S_{\text{jump-start}} = P_\perp + \frac{ip_1 - k(\lambda) - \alpha_1^2 \frac{1}{\lambda - \lambda_1^\Lambda}}{ip_1 + k(\lambda) + \alpha_1^2 \frac{1}{\lambda - \lambda_1^\Lambda}} P_1^\Lambda. \tag{56}
\]

It corresponds to the one-dimensional solvable model of the junction, obtained via attachment an appropriate inner structure to the vertex, see Fig. [2]. This approximate expression for the scattering matrix can be obtained via imposing on the Scattering Ansatz a \(\lambda\)-dependent boundary condition at the vertex, see a discussion in \[43\]. Unfortunately this boundary condition does not correspond to a
self-adjoint operator, so that it can’t be interpreted in terms of Quantum Mechanics, the same as prominent Wigner boundary condition, see [75]. We are also able to represent the scattering matrix with use of a single Blaschke-factor:

\[ S_{\text{approx}}(\lambda) = P_1^+ + \left[ \frac{ip(\lambda - \lambda_1^\Lambda) - \alpha_1^2}{ip(\lambda - \lambda_1^\Lambda) + \alpha_1^2} \right] P_1^\Lambda \equiv P_1^+ + \Theta_1^\Lambda(\lambda) P_1^\Lambda. \] (57)

Notice that the scalar Blaschke-factor \( \Theta_1^\Lambda \) is close to \(-1\) on the essential spectral interval

\[ \Delta_T : \{ \lambda : |\lambda - \lambda_1^\Lambda| \leq 2m^* \kappa T \hbar^{-2} < \alpha_1^2 p^{-1}(\lambda_1^\Lambda) \}, \]

for low temperature \( T \), and it is close to 1 on the complement. For thin junction and low temperature the boundary condition can be reduced to Datta-type boundary condition, see below, formula (64) represented in terms of boundary currents of the resonance eigenfunction of the Intermediate Hamiltonian.

Once we already developed the compensation procedure based on the representation of the Intermediate DN-map in terms of classical DN-map, we can do one more step, expressing the approximate scattering matrix (55) in spectral terms of the unperturbed operator \( L_{\text{int}} \) on the vertex domain \( \Omega_{\text{int}} \), under assumption that it has a single resonance eigenvalue \( \lambda_1 \in \Delta_T \subset \Delta \),

\[ L_{\text{int}} \varphi_1 = \lambda_1 \varphi_1. \]

Then, for thin junction, the intermediate Hamiltonian also has a simple eigenvalue near to \( \lambda_1 \). We assume that the major part of the correcting term \( K^\Delta \) in the corresponding rational approximation of the DN-map of \( L_{\text{int}} \) is defined by a finite sum of polar terms and a regular term \( M_{\text{reg}} = K_{++}^\Delta - K_{+-}^\Delta + \frac{I}{\lambda_1^\Lambda + K_{--}^\Delta} \), see (3.1)

\[ K^\Delta = \sum_{s=2}^{M} \frac{I}{\lambda - \lambda_s} \frac{\partial \varphi_s}{\partial n} \langle \frac{\partial \varphi_s}{\partial n} + M_{\text{reg}}, \]

Figure 7. 1-d model of T-junction
\[
DN(\lambda) = \frac{I}{\lambda - \lambda_1} \frac{\partial \varphi_1}{\partial n} \frac{\partial \varphi_1}{\partial n} + \sum_{s=2}^{s=M} \frac{I}{\lambda - \lambda_s} \frac{\partial \varphi_s}{\partial n} \frac{\partial \varphi_s}{\partial n} =: DN^\Delta + K^\Delta,
\]
\[
T = \varphi_1 \langle \frac{\partial \varphi_1}{\partial n} \rangle, \quad J = P_+ - K_{++} K_{--}^{-1} [I + K_{--} K_{--}^{-1}]^{-1} P_-
\]

Hereafter we neglect the contribution from higher terms of the geometrically convergent series
\[
[I + K_{--} K_{--}^{-1}]^{-1} P_+ \approx I_+ = P_+
\]
\[
J = P_+ - K_{++} K_{--}^{-1} \approx P_+ - \sum_{s=2}^{s=M} \frac{I}{\lambda - \lambda_s} P_+ \frac{\partial \varphi_s}{\partial n} \langle K_{--}^{-1} \frac{\partial \varphi_s}{\partial n} \rangle
\]

Then, with only terms containing \(K_{--}^{-1}\) taken into account, we obtain for \(M\), based on Theorem 3.1, an approximate expression for the essential spectral interval \(\Delta\)
\[
Q(\lambda) = \varphi_1 \langle \frac{\partial \varphi_1}{\partial n} \rangle K_{--}^{-1} [I + K_{--} K_{--}^{-1} P_+]^{-1} \frac{\partial \varphi_1}{\partial n} \langle \varphi_1 \biggl( \frac{\partial \varphi_1}{\partial n} \biggr) K_{--}^{-1} \frac{\partial \varphi_1}{\partial n} \rangle.
\]

For “very thin” junction one can neglect even first order terms containing \(K_{--}^{-1}\), everywhere, except the expression staying in the denominator, and obtain from \(58\) a simpler approximate formula:
\[
\mathcal{M}_{\text{approx}} = K_{++}^\Delta - K_{--}^\Delta K_{--}^\Delta +
\]
\[
(P_+ - K_{++} K_{--}^{-1}) \frac{\partial \varphi_1}{\partial n} \bigg|_{\Gamma} \frac{I}{\lambda - \lambda_1 + \langle K_{--}^{-1} \frac{\partial \varphi_1}{\partial n} \rangle_{\Gamma}} \langle (P_+ - K_{--} K_{--}^{-1}) \frac{\partial \varphi_1}{\partial n} \rangle_{\Gamma}.
\]

\[\text{(58)}\]

For “very thin” junction one can neglect even first order terms containing \(K_{--}^{-1}\), everywhere, except the expression staying in the denominator, and obtain from \(58\) a simpler approximate formula:
\[
\mathcal{M}_{\text{thin}} = K_{++}^\Delta + P_+ \frac{\partial \varphi_1}{\partial n} \bigg|_{\Gamma} \frac{I}{\lambda - \lambda_1 + \langle K_{--}^{-1} \frac{\partial \varphi_1}{\partial n} \rangle_{\Gamma}} \langle P_+ \frac{\partial \varphi_1}{\partial n} \rangle_{\Gamma} =:
\]
\[
K_{++}^\Delta + \alpha_1^2 \frac{P_1^Q}{\lambda - \lambda_1^Q}
\]

\[\text{(59)}\]

where
\[
P_1^Q = e_1^Q \langle e_1^Q, e_1^Q \rangle = \alpha_1^{-1} P_+ \frac{\partial \varphi_1}{\partial n} \bigg|_{\Gamma}, \quad \alpha_1 = \| P_+ \frac{\partial \varphi_1}{\partial n} \|^2, \quad \lambda_1^Q = \lambda_1 - \langle \frac{\partial \varphi_1}{\partial n} \rangle_{\Gamma} K_{--}^{-1} \frac{\partial \varphi_1}{\partial n} \rangle_{\Gamma}.
\]

This implies an approximate formula for the scattering matrix on the major part of the essential spectral interval \(\Delta_R\) for low temperature, once the junction is thin on the open channel
\[
p^2(\Lambda) = |\Lambda - (\pi^2 \delta^2 + V_0)| > \| K_{++}^\Delta \|.
\]

\[\text{(60)}\]

\(^3\text{Roughly speaking, on a complement of a certain small neighborhood of the zero } \lambda_1^Q \text{ of the denominator.}\)
Notice that arising of the shape of the resonance eigenfunction of the unperturbed operator \( L_{\text{int}} \) in the corresponding approximate jump-start formula (61) for the scattering matrix corresponds to folklore observation of physicists, that the eigenfunctions react to perturbation slower that the eigenvalues. To derive the jump-start approximation for the scattering matrix, denote \( \sqrt{\lambda - \pi^2 \delta^{-2} - V_\delta} =: p \). Then we obtain on \( \Delta_T \), similarly to Theorem 4.1:

\[
S(\lambda) \approx P_1^\perp + \frac{ip - k - \frac{\alpha_1^2}{\lambda - \lambda_1^2}}{ip + k + \frac{\alpha_1^2}{\lambda - \lambda_1^2}} P_1 =: S_{\text{jump-start}}^Q. \tag{61}
\]

In the case when \( \lambda_1^Q \approx \Lambda \) we can replace on \( \Delta_T \) the Blaschke factor in front of \( P_1 \) by \(-1\), which implies on \( \Delta_T \), for sufficiently low temperature:

\[
S_{\text{jump-start}}^Q(\lambda) \approx P_1^\perp - P_1 \equiv S_{\text{Datta}} \tag{62}
\]

When modeling the quantum network by a one-dimensional graph, one can attempt to define a boundary condition at the vertex which implies the scattering matrix (62). Indeed, forming the component \( \Psi_{+}^\perp(\nu) \) of the scattering Ansatz based on (62), we see the the boundary values of the Ansatz

\[
\Psi_{+}(x, \nu) = e^{iK_{+}x} \psi_{+} + e^{-iK_{+}x} S_{\nu}
\]

satisfy the following boundary condition, similar to one suggested in [13]:

\[
\Psi_{+}(0, \nu) = 2P_1^\perp \psi_{+}(0, \nu) = 2P_1 \psi_{+}(0, \nu).
\]

In terms of the components \( \Psi_{+}^n(0, \nu), \frac{d}{dx} \Psi_{+}^n(0, \nu) \) of the boundary values of the Ansatz on the bottom sections \( \Gamma_n \) of the wires and with use of the components of the boundary currents \( \vec{\psi}_{1} = \{\psi_{1}^n\}_{n=1}^{N} \)

\[
P_+ \frac{\partial \varphi_1}{\partial n} \bigg|_{\Gamma_n} = \psi_{1}^n \tag{63}
\]

we obtain: \( \langle \vec{\psi}, \Psi_{+}(0, \nu) \rangle = 0, \frac{d}{dx} \Psi_{+}(0, \nu) \parallel \vec{\psi} \), or

\[
\langle \vec{\psi}, \Psi_{+}(0, \nu) \rangle = \sum_{n}^{N} \Psi_{+}^n(0, \nu) \vec{\psi}^n = 0,
\]

\[
\frac{d}{dx} \Psi_{1}^\perp(0, \nu) = \frac{d}{dx} \Psi_{2}^\perp(0, \nu) = \ldots = \frac{d}{dx} \Psi_{n}^\perp(0, \nu) = \ldots = \frac{d}{dx} \Psi_{N}^\perp(0, \nu)
\]

**Example 4: asymmetric T-junction** Consider a two-dimensional quantum network \( \Omega \) constructed as a simplest asymmetric T-junction of three straight semi-infinite quantum wires width \( \pi/2 \) attached as shown in Fig. 8 to the quantum well - the square \( \Omega_{\text{int}} \): \( 0 < x < \pi, 0 < y < \pi \) on \( x, y \)-plane. The role of the one-electron Hamiltonian on \( \Omega \) is played the Dirichlet Laplacian. The spectrum of the

\footnote{but not yet equivalent, see an extended discussion below, in next subsection.}
corresponding unperturbed Hamiltonian on the quantum well is discrete and the
eigen-pairs e.g.

\[ \lambda_1 = 2 : \varphi_{1,1} = \frac{2}{\pi} \sin x \times \sin y; \]

\[ \lambda_2 = \lambda_3 = 5; \varphi_{1,2} = \frac{2}{\pi} \sin x \times \sin 2y \text{ and } \varphi_{2,1} = \frac{2}{\pi} \sin 2x \times \sin y; \]

\[ P_5 = P_{1,2} + P_{2,1}, \quad P_{1,2} = \varphi_{1,2} \quad \langle \varphi_{1,2} : P_{2,1} = \varphi_{2,1} \rangle \langle \varphi_{2,1} ; \]

\[ \lambda_4 = 8; \varphi_{2,2} = \frac{2}{\pi} \sin 2x \times \sin 2y; \quad P_8 = P_{2,2} = \varphi_{2,2} \quad \langle \varphi_{2,2} ; \]

\[ \lambda_5 = \lambda_6 = 10; \varphi_{1,3} = \frac{2}{\pi} \sin x \times \sin 3y \text{ and } \varphi_{3,1} = \frac{2}{\pi} \sin 3x \times \sin y; \ldots \]

\[ \lambda_6 = \lambda_7 = 13; \varphi_{2,3} = \frac{2}{\pi} \sin 2x \times \sin 3y \text{ and } \varphi_{3,2} = \frac{2}{\pi} \sin 3x \times \sin 2y; \ldots \]

\[ \ldots \ldots \]

are obtained via separation of variables. We choose the basic spectral interval
\[ \Delta = [4,6], \] so that there is only one multiple eigenvalue \( \lambda_2 = \lambda_3 = 5 \) of \( L_{\text{int}} \) on
that interval, and use the approximate formula \(59\) for \(M\). The normal boundary current \(J_{1,2}\) of the resonance eigenfunctions \(\varphi_{1,2}\) and \(\varphi_{2,1}\) is calculated as

\[
J_{1,2} = \begin{pmatrix}
\frac{\partial \varphi_{1,2}}{\partial n} \\
\frac{\partial \varphi_{1,2}}{\partial n} \\
\frac{\partial \varphi_{1,2}}{\partial n}
\end{pmatrix} = \begin{pmatrix}
-\frac{2}{\pi} \sin 2y \\
\frac{4}{\pi} \sin x \\
-\frac{2}{\pi} \sin 2y
\end{pmatrix},
\]

\[
J_{2,1} = \begin{pmatrix}
\frac{\partial \varphi_{2,1}}{\partial n} \\
\frac{\partial \varphi_{2,1}}{\partial n} \\
\frac{\partial \varphi_{2,1}}{\partial n}
\end{pmatrix} = \begin{pmatrix}
\frac{4}{\pi} \sin y \\
-\frac{2}{\pi} \sin 2x \\
-\frac{4}{\pi} \sin y
\end{pmatrix}.
\]

The spectrum of the unperturbed Hamiltonian on the wires is absolutely-continuous and has a band structure, with thresholds \(\{l^2\}, l = 1, 2, 3 \ldots\) separating the spectral bands. The multiplicity of the continuous spectrum jumps up by three units on each threshold. We assume that the first spectral band \(\Delta_1 = [4, 16]\) is the conductivity band. The entrance subspace of the open channel is spanned by the inferior cross-section eigenfunctions \(e_{s,1}^+ = (4/\pi)^{1/2} \sin 2x_s^+\), \(s = 1, 2, 3\) on the bottom cross-section \(\Gamma_s = [0 < x_s^+ < \pi/2], s = 1, 2, 3\). The entrance subspace of closed channels is the linear hull of the superior cross-section eigenfunctions \(e_{s,l}^\perp = (4/\pi)^{1/2} \sin 2lx_s^+, s = 1, 2, 3, \) with \(l = 2, 3, \ldots\). We will calculate the approximate scattering matrix (jump-start) of the thin junction based on the approximate formulae for \(53, 59\). The approximate eigenvalues of the intermediate Hamiltonian are found as zeros of the denominator \(d(\lambda)\) represented as a \(2 \times 2\) matrix with respect to the basis \(\varphi_{1,2}, \varphi_{2,1}\):

\[
d(\lambda) = \begin{pmatrix}
\lambda - 5 & 0 \\
0 & \lambda - 5
\end{pmatrix} +
\begin{pmatrix}
\langle P_- \frac{\partial \varphi_{1,2}}{\partial n} |_{\Gamma} K_-^{-1} P_- \frac{\partial \varphi_{1,2}}{\partial n} |_{\Gamma} \rangle \\
\langle P_- \frac{\partial \varphi_{2,1}}{\partial n} |_{\Gamma} K_-^{-1} P_- \frac{\partial \varphi_{2,1}}{\partial n} |_{\Gamma} \rangle
\end{pmatrix}.
\]

Taking into account only components of the currents in the second spectral channel

\[
K_- \frac{\partial \varphi_{1,2}}{\partial n} |_{\Gamma} \approx e_{s,2} \langle \frac{\partial \varphi_{1,2}}{\partial n} |_{\Gamma} e_{s,2} \rangle
\]

and introducing the following notations for the integrals

\[
2 \int_0^{\pi/4} \sin 2x \sin 4xdx = \frac{2}{3} =: \alpha,
\]

\[
\int_0^{\pi/2} \sin x \sin 4xdx = -\frac{4}{15} =: \gamma, \; \alpha + \gamma = \frac{2}{5} =: \beta,
\]
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we represent the denominator \((\lambda - 5)^{-1}\) and the inverse \([d(\lambda)]^{-1}\) as

\[
d(\lambda) = \begin{pmatrix} \lambda - 5 & 0 \\ 0 & \lambda - 5 \end{pmatrix} + \frac{\pi}{4\sqrt{16 - \lambda}} \begin{pmatrix} \alpha^2 & -\alpha \beta \\ -\alpha \beta & \beta^2 \end{pmatrix} = (\lambda - 5) \frac{1}{\alpha^2 + \beta^2} \begin{pmatrix} \beta \\ \alpha \end{pmatrix} \begin{pmatrix} \beta \\ \alpha \end{pmatrix}
\]

\[
\left(\lambda - 5 + \frac{\pi}{4\sqrt{16 - \lambda}}\right) \frac{1}{\alpha^2 + \beta^2} \begin{pmatrix} -\alpha \\ \beta \end{pmatrix} \begin{pmatrix} -\alpha \\ \beta \end{pmatrix}.
\]

\[
[d(\lambda)]^{-1} =: P_5 + \frac{P_{5-\delta_Q}}{\lambda - 5 + \delta_Q}, \tag{68}
\]

with \(\delta_Q = \pi \frac{[\alpha^2 + \beta^2]}{4 \sqrt{16 - \lambda}}\). Here \(K_1\) is substituted by the contribution \(\frac{4}{\pi} \sin 4x\sin 2y\) from the second spectral branch in the wires.

If the scaled Fermi-level is 5, then the corresponding multiple resonance eigenvalue of \(L_{int}\) is split into pair of eigenvalues \(\lambda_1^\ast = 5\), \(\lambda_2^\ast = 5 - \frac{\pi}{4\sqrt{16 - 5}}\), and the jump-start approximation of the scattering matrix can be calculated in terms of \(P_+\) -

projections of the boundary currents of the resonance eigen functions \(\varphi_{1,2}, \varphi_{2,1} :=

\[
P_+ \frac{\partial \varphi_{1,2}}{\partial n} \bigg|_\Gamma = P_+ J_{1,2} = \begin{pmatrix} P_+ \frac{\partial \varphi_{1,2}}{\partial n} \\ \Gamma_1 \\ 0 \end{pmatrix} = \begin{pmatrix} P_+ \frac{\partial \varphi_{2,1}}{\partial n} \\ \Gamma_2 \\ P_+ \frac{\partial \varphi_{2,1}}{\partial n} \end{pmatrix} \Gamma_3
\]

\[
\begin{pmatrix} -\frac{4}{\pi} \sin 2x_1 \int_{\Gamma_1} \sin 2x_1 \sin 2y d\Gamma_1 \\ \frac{8}{\pi} \sin 2x_2 \int_{\Gamma_2} \sin 2x_2 \sin x d\Gamma_3 \\ -\frac{4}{\pi} \sin 2x_3 \int_{\Gamma_3} \sin 2x_3 \sin 2y d\Gamma_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 16\sqrt{2}/3\pi^2 \\ -4/\pi \end{pmatrix} =: \begin{pmatrix} 2 \sqrt{2}/\pi \sin 2x_2 \psi_{1,2} \\ \end{pmatrix}
\]

\[
P_+ \frac{\partial \varphi_{2,1}}{\partial n} \bigg|_\Gamma = P_+ J_{2,1} = \begin{pmatrix} P_+ \frac{\partial \varphi_{2,1}}{\partial n} \\ \Gamma_1 \\ P_+ \frac{\partial \varphi_{2,1}}{\partial n} \end{pmatrix} \Gamma_3
\]

\[
\begin{pmatrix} 0 \\ 16\sqrt{2}/3\pi^2 \\ -4/\pi \end{pmatrix} = \begin{pmatrix} P_+ \frac{\partial \varphi_{2,1}}{\partial n} \\ \Gamma_1 \\ P_+ \frac{\partial \varphi_{2,1}}{\partial n} \end{pmatrix} \Gamma_3
\]
The exponent $K_+$ of the first (open) channel is represented as $K_+ (\lambda) = \sqrt{\lambda - 4P_+}$, where the projection $P_+$ onto the entrance subspace of open channels plays the role of unity $I_+ = I_1 + I_2 + I_3$ in $E_+$ and is represented as

$$P_+ = 4/\pi \left[ (\sin 2x_1^+) (\sin 2x_1^+ + \sin 2x_2^+) (\sin 2x_1^+ + \sin 2x_3^+) \right].$$

Then taking into account that the contribution $K_{++}$ from the major polar part of $K \approx P_+8/\pi$ is

$$K_{++} \approx \frac{16}{\pi^3} \frac{\sin 2x_3^+ (\sin 2x_3^+)}{\lambda - 8} = \frac{2}{\sqrt{\pi}} \sin 2x_3^+ \left( \frac{2}{\sqrt{\pi}} \sin 2x_3^+ \right),$$

and omitting the vector factors $2/\sqrt{\pi} \sin 2x_1^+$ and $2/\sqrt{\pi} \sin 2x_1^+$ on the right and left side of the jump-start scattering matrix,

$$S_{\text{jump-start}} = \frac{ipI_+ - \frac{4f_s}{\lambda - 8} - \left( \begin{array}{c} \psi_1^2 \\ \psi_2 \end{array} \right) \left[ \begin{array}{cc} P_{\lambda - 8} & P_{\lambda - 8} \delta Q \\ \lambda - 8 + 8\delta Q \end{array} \right] \left( \begin{array}{c} \psi_1^2 \\ \psi_2 \end{array} \right) }{ipI_+ + \frac{4f_s}{\lambda - 8} + \left( \begin{array}{c} \psi_1^2 \\ \psi_2 \end{array} \right) \left[ \begin{array}{cc} P_{\lambda - 8} & P_{\lambda - 8} \delta Q \\ \lambda - 8 + 8\delta Q \end{array} \right] \left( \begin{array}{c} \psi_1^2 \\ \psi_2 \end{array} \right) }.$$

For better approximation of the scattering matrix we should use better approximation for $K_-, K_\Delta$.

### 4.2. Symmetric junction.

The Datta-type boundary condition (64) does not coincide with the original Datta-Das Sarma boundary condition (1, 2), suggested in [13], because the phenomenological Datta-Das Sarma boundary condition was suggested for a T-junction which is symmetric with respect to the left-right reflection. The resonance concept of the conductance permits to derive, for a symmetric junction, the original Datta-Das Sarma condition and interpret the phenomenological parameter $\beta$.

Consider a symmetric junction $\Omega$ consisting of a square $(0, \pi) \times (0, \pi)$, and the quantum wires width $\pi/2$, attached in the middle of the sides $\Gamma_1, \Gamma_2, \Gamma_3$, see (4). The role of the one-electron Hamiltonian is played by the Laplacian on $\Omega$ with zero boundary conditions. Similarly to above example we assume that the electrons are supplied from the second wire, in the first spectral channel. We assume that the scaled Fermi level is $\Lambda = 10$ and the conductivity band is $4 \leq$
\( \lambda \leq 16 \), the eigenvalues of \( L_{\text{int}} \) embedded into the conductivity band are \( \lambda_0 = 5 \), \( \lambda_1 = 8 \), \( \lambda_2 = 10 \), \( \lambda_3 = 13 \). The corresponding eigenfunctions of \( L_{\text{int}} \) are found in previous subsection via separation of variables, see (65). The role of the resonance eigenfunctions is played by \( \varphi_{1,3}, \varphi_{3,1} \), with the eigenvalue \( \lambda_5 = \lambda_6 = 10 \). We also use the symmetric and antisymmetric linear combinations of them

\[
2^{-1/2}[\varphi_{1,3} + \varphi_{3,1}] =: \varphi_s, \quad 2^{-1/2}[\varphi_{1,3} - \varphi_{3,1}] =: \varphi_a.
\]

We denote the corresponding boundary currents as

\[
\frac{\partial \varphi_s}{\partial n} \bigg|_\Gamma =: J_s, \quad \frac{\partial \varphi_a}{\partial n} \bigg|_\Gamma =: J_a
\]

and consider the projections of them \( P_+ J_{\text{sym}}, P_+ J_{\text{asym}} \) onto the entrance space of the first (open) channel. We assume that the temperature is low, so that the role of an essential spectral interval is played by \( \Delta_T = [9, 11] \). Then the eigenfunctions and eigenvalues of the intermediate Hamiltonian can be found based on Theorem 3.1, taking into account the approximate calculation of the potential \( Q(\lambda) \) of \( L^\Delta(\lambda) \):

\[
Q(\lambda) \approx \langle \varphi_{1,3}, \varphi_{3,1} \rangle_D \langle \varphi_{1,3}, \varphi_{3,1} \rangle,
\]

with

\[
D = \begin{pmatrix}
\langle P_{-} \frac{\partial \varphi_{1,3}}{\partial n} \bigg|_\Gamma & K^{-1} P_{-} \frac{\partial \varphi_{1,3}}{\partial n} \bigg|_\Gamma \\
\langle P_{-} \frac{\partial \varphi_{3,1}}{\partial n} \bigg|_\Gamma & K^{-1} P_{-} \frac{\partial \varphi_{3,1}}{\partial n} \bigg|_\Gamma \\
\langle P_{+} \frac{\partial \varphi_{1,3}}{\partial n} \bigg|_\Gamma & K^{-1} P_{+} \frac{\partial \varphi_{1,3}}{\partial n} \bigg|_\Gamma \\
\langle P_{+} \frac{\partial \varphi_{3,1}}{\partial n} \bigg|_\Gamma & K^{-1} P_{+} \frac{\partial \varphi_{3,1}}{\partial n} \bigg|_\Gamma
\end{pmatrix},
\]

and thus neglecting \( Q \) in the case of thin networks. Hence, in the first order approximation, the perturbed eigenvalues of the Intermediate Hamiltonian remain the same: \( \lambda_{5}^Q = \lambda_{6}^Q = 10 \). Due to reflection symmetry of the junction there are two eigenfunctions of the Intermediate Hamiltonian which correspond to the eigenvalue multiplicity 2 obtained based on Theorem 3.1. The corresponding eigenfunctions and the projections of the normal currents onto \( E_+ \) are respectively symmetric and anti-symmetric:

\[
\psi_{a,s} = P_+ \frac{\partial \varphi_{a,s}}{\partial n} \bigg|_{P_+ \frac{\partial \varphi_{a,s}}{\partial n}}^{-1}
\]

\[
\sqrt{2 + \gamma^2} \begin{pmatrix}
1 \\
-1
\end{pmatrix}
\]

and the orthogonal complement in \( E_+ \) is spanned by the vector

\[
\gamma \sqrt{4 + 2\gamma^2} \begin{pmatrix}
-2/\gamma \\
1
\end{pmatrix} =: \beta \begin{pmatrix}
1 \\
\gamma
\end{pmatrix},
\]

with \( \beta = -2/\gamma \). In the first order approximation \( K \) can be substituted by the contribution from the nearest eigenvalue \( \lambda_4 = 8 \), and hence \( K_{++} = k = 0 \).
The intermediate DN-map is represented, due to Theorem 3.1 by the formula

\[ M = \frac{\alpha_2^2 P_a + \alpha_2^2 P_s}{\lambda - \lambda_Q^2} + K_{++} \approx \frac{\alpha_2^2 P_a + \alpha_2^2 P_s}{\lambda - 10}, \]

where \( P_a = \langle e_a, P_a e_a \rangle \) and \( P_s = \langle e_s, P_s e_s \rangle \). Then denoting by \( P_\perp := P_+ - [P_a + P_s] =: P_+ - P_Q \), we represent the scattering matrix of the symmetric junction as

\[ S = P_\perp \frac{ipP_Q - \alpha_2^2 P_a + \alpha_2^2 P_s}{ipP_Q + \alpha_2^2 P_a + \alpha_2^2 P_s} \]

Here the role of the scalar Blaschke factor \( \Theta_1 \) in (57) is played by the 2 \( \times \) 2 matrix

\[ \Theta = \frac{ip(\lambda - \lambda_Q^2)P_Q - [\alpha_2^2 P_a + \alpha_2^2 P_s]}{ip(\lambda - \lambda_Q^2)P_Q + [\alpha_2^2 P_a + \alpha_2^2 P_s]}. \]

The matrix \( \Theta \) for low temperature is close to \(-P_Q\) on the corresponding small essential spectral interval \( \Delta_\tau \) centered at \( \lambda_Q^2 \). Then the scattering matrix is represented as

\[ S = P_\perp^2 - P_Q, \]

with the pair of complementary projections \( P_\perp^2 \) and \( P_Q \), \( \dim P_\perp^2 = 1 \), \( \dim P_Q = 2 \). Scattering Ansatz on the model graph

\[ \Psi = e^{ipP_1 x}e + e^{-ipP_2 x}S e \]

satisfies the following boundary condition at the vertex \( x = 0 \):

\[ \Psi(0) = (I + S)e = 2P_\perp^2 e, \quad \Psi'(0) = ipP_+ (I - S)e = 2ipP_Q e. \]

Taking into account that \( \dim P_\perp^2 = 1 \), \( \dim P_Q = 2 \), we can re-write the previous formulae as boundary conditions imposed on the Ansatz:

\[ P_\perp^2 \tilde{\psi}(0) = 0, \quad \tilde{\psi}(0) \text{ is parallel to } P_\perp^2 e \]

\[ \langle e_1^+, \psi'(0) \rangle = 0, \quad e_1^+ = \frac{\psi_1(0)}{e_1^+}, \quad e_2^+ = \frac{\psi_2(0)}{e_2^+}, \quad e_3^+ = \frac{\psi_3(0)}{e_3^+}. \]

(71)

where \( P_\perp^2 =: e_1^+ \langle e_1^+, e_1^+ \rangle = (e_1^+, e_2^+, e_3^+) = (2 + \beta^2)^{-1/2}(1, \beta, 1) \). This condition coincides with the original Datta-das-Sarma boundary condition, see (112). Our analysis reveals the meaning of the phenomenological parameter \( \beta \).

5. A solvable model of a thin junction

Generally, a Schrödinger operator with non-constant coefficients or one in a non-standard domain rarely admits spectral analysis in explicit form. For qualitative analysis of quantum systems the Schrödinger operator often is substituted by a solvable model, constructed by the von Neumann operator extension technique, see for instance [7, 14, 5] and an extended list of references in [4]. In particular, the substitution of the network by a proper one-dimensional graph, with special
boundary conditions at the vertices, looks like a convenient tool for the qualitative analysis of the Schrödinger equation on the network. Unfortunately the estimation of the error caused by the substitution of the network by the corresponding graph is difficult. Shrinking of a “fattened graph” \( \Omega_\delta \) to one-dimensional graph was studied in numerous papers, see for instance \cite{36,37}. The authors considered a compact network \( \Omega_\delta \) constructed of the vertex domains \( \Omega_{\text{in}} \), with the diameter proportional to \( \delta^\alpha \), \( 0 < \alpha < 1 \) and several finite leads \( \omega^m \), width \( \delta \), joining them to each other. In \cite{66} they developed, based on \cite{74,67}, a variational technique for description of the asymptotic behavior of the discrete spectrum of the Schrödinger operator on the quantum network \( \Omega_\delta \) of various grades \( \alpha \) of thinness. It appeared that the (discrete) spectrum of the Laplacian on the compact shrinking “fattened graph” \( \Omega_\delta \) tends to the spectrum of the Laplacian on the corresponding one-dimensional graph but with different boundary conditions at vertices depending on the speed of shrinking: the Kirchhoff boundary conditions at the nodes, in the case of “small protrusion” \( 1/2 < \alpha < 1 \), or the homogeneous Dirichlet boundary conditions, in case of “large protrusion”, \( 0 < \alpha < 1/2 \), see \cite{37}, theorems 1,2,3.

In this section we consider a thin quantum networks with small protrusion \( \alpha = 1 \), assuming diam \( \delta << \text{diam} \Omega_{\text{in}} \). We will construct a quantitatively consistent solvable model of the quantum network, in the form of a star-graph with a vertex supplied with inner space and appropriate vertex Hamiltonian. The scattering matrix of the properly fitted model serves as a local approximation - on a certain “essential” spectral interval \( \Delta \) - of the scattering matrix of the original network. In contrast to the quoted above results for compact networks, where the wave-functions are obtained based on the variational approach, we use Dirichlet-to-Neumann map \( DN^\Lambda \) of an intermediate Hamiltonian \( L_\Lambda \), to derive an explicit formula for the scattered waves on the original network, see \cite{22}. The scattering matrix of the star-graph model is obtained via replacement of \( M \) in \cite{22} by the corresponding rational approximation on \( \Delta \), based on Theorem \ref{thm:3.1}. This defines all parameters of the model in terms of spectral characteristics of \( L_\Lambda \). In course of construction and fitting of the solvable star-graph model we also define the energy-dependent boundary conditions at the vertex for the Schrödinger equation on the graph. In the simplest case when only one resonance eigenvalue \( \lambda_0 \) of the intermediate Hamiltonian is present on \( \Delta \), this condition depends linearly on the spectral parameter, and is parametrized by coordinates \( \Re k_0, \Im k_0 \) of the corresponding resonance.

Note that in \cite{33} an algorithm for construction of the scattering matrix of the quantum graph of the scattering matrices of star-shaped elements is described and, in \cite{25} a convenient formula for the scattering matrix of the star-graph in terms of the boundary parameters at the vertex is suggested. For extended discussion of properties of star graphs see \cite{29,30}.

The star-graph solvable model of the thin junction will be constructed as a finite-dimensional perturbation of an orthogonal sum of the non-perturbed Hamiltonian \( l_\Lambda \) in the open channels and a finite matrix \( A \) acting in the inner space of the vertex.
We will choose the parameters of the model such that the model scattering matrix coincides with the few-pole approximation $S_\Delta$ of the complete scattering matrix $S$. Then the constructed model will be automatically fitted (i.e. quantitatively consistent). We assume that the spectral variable is scaled such that original the Schrödinger equation on the wires is just $-\Delta u + V u = \lambda u$. The scattering Ansatz of the model in open channels satisfies on the wires $\omega$ the same equation as the scattering Ansatz on the original network

$$l_\Delta := -\frac{d^2 U_\omega}{dx^2} + \sum_{s,m} \frac{\pi^2}{s^2} P_s^m U + V u := \lambda , \lambda \in \Delta , \ U = U_\omega = (u^1, u^2, \ldots u^M).$$

(72)

We assume that the Schrödinger equation on the quantum well $\Omega_{int} = \Omega_0$, with the same spectral parameter, is represented as

$$L_0 u := -\Delta u + V u = \lambda u,$$

with a corresponding effective mass $\mu_0$. We assume that the Intermediate relative DN-map, $P_\Gamma^\beta \frac{\partial u}{\partial n} \big|_\Gamma = DN u$, with respect to $\Gamma$, is calculated and the corresponding rational approximation is selected. Then the construction of the vertex part of the model will be done with a major change of the original Intermediate Hamiltonian. For thin networks an auxiliary spectral interval $\Delta$ is selected inside $\Delta_1 = [\pi^2, 4\pi^2]$, and hence does not overlap with the continuous spectrum of the intermediate Hamiltonian $L_\Delta$. Only a finite number $N$ of eigenvalues of the intermediate operator are situated on $\Delta$. Then substitution of $\mathcal{M}$ on $\Delta$ by the rational approximation $\mathcal{M}_\Delta$ may cause only a minor and controllable error. Now we will prove that there exist a finite-dimensional perturbation of the operator $l_\Delta \oplus A$ such that the scattering matrix of the perturbed operator coincides with $S_\Delta$. The perturbation will be constructed via operator restriction-extension procedure applied to the orthogonal sum $l_\Delta \oplus A$, where $A$ is an $N \times N$ Hermitian matrix : $E_A \rightarrow E_A$, $\dim E_A = N$. The parameters of the model will be properly selected to fit the spectral data of the Intermediate Hamiltonian on the original quantum network, within the auxiliary spectral interval $\Delta$.

Assume that the positive matrix $A$ is defined by its spectral decomposition

$$A = \sum_r \alpha^2_r P_r.$$

Here $\alpha^2 > 0$ are eigenvalues of $A$, and $P_r = \nu_r \langle \nu_r$ are the corresponding orthogonal spectral projections. The eigenvalues and the boundary parameters $\beta$ of the model, see below (82), will be defined later, based on comparison of the scattering matrix of the model with the essential scattering matrix

$$S_\Delta = [iK_+ + DN\Delta]^{-1}[iK_- - DN\Delta].$$

(73)
Then the adjoint operator \( l_0^* \) is defined on \( W^2_2(E_+, R_+) \), and the boundary form of it is calculated via integration by parts:

\[
\mathcal{J}_i(U, V) = \langle l_0^* U, V \rangle - \langle U, l_0^* V \rangle = \langle U'(0), V(0) \rangle - \langle U(0), V'(0) \rangle,
\]

(74)

where \( U(0), V(0) \in E_+ \) and the derivatives are taken in the outgoing direction on \( \Gamma \) with respect to \( \Omega_n \).

Restriction of the matrix \( A \) is equivalent to selection of the deficiency subspace for the given value \( i \) of the spectral parameter. Choose a generating subspace \( N_i, \bigoplus_{k>0} A^k N_i = E_+ \) such that \( \frac{A+iI}{A-iI} N_i \cap N_i = 0 \), \( \dim N_i = d \), set \( D_0^A = (A - iI)^{-1} (E_+ \oplus N_i) \) and define the restriction of the inner Hamiltonian as \( A \rightarrow A_0 = A|_{D_0^A} \). We develop the extension procedure for general \( N_i \) and fit it later based on spectral data of the intermediate operator, see Theorem 4.1, 4.2. In our construction \( N_i \subset E_+ \) will play a role of the deficiency subspace at the spectral point \( i \), \( \dim N_i = d \), \( 2d \leq N \) and the dual deficiency subspace is \( N_{-i} = \frac{A+iI}{A-iI} N_i \).

The domain of the restricted operator \( A_0 \) is not dense in \( E_+ \), because \( A \) is bounded. Nevertheless, since the deficiency subspaces \( N_{\pm i} \) do not overlap, the extension procedure for the orthogonal sum \( l_0 \oplus A_0 \) can be developed. We will do it here with use of the symplectic formalism, see for instance [53]. In this case the “formal adjoint” operator for \( A_0 \) is defined on the defect \( N_i + N_{-i} := N \) by the von Neumann formula: \( A_0^+ e \pm i e = 0 \) for \( e \in N_{\pm i} \). Then the extension is constructed, see lemmas 3.1-3.4 below, via restriction of the formal adjoint onto a certain plane in the defect where the boundary form vanishes (a “Lagrangian plane”). According to the classical von Neumann construction all Lagrangian planes are parametrized by isometries \( V : N_i \rightarrow N_i \) in the form

\[
T_V = (I - V) N_i.
\]

In case when the deficiency subspaces do not overlap, the corresponding isometry is admissible, and, according to [34] there exist a self-adjoint extension \( A_V \) of the restricted operator \( A_0 \). We construct this extension based on the following

**Lemma 5.1.** The lagrangian plane \( T_V \) in the defect forms a non-zero angle with the domain \( D_0^A \) of the restricted operator \( A_0 \).

**Proof** Indeed, if \( A_V \) is the extension, then on the \( T_V \) it coincides with the restriction of the formal adjoint, and on the domain \( D_0^A \) it coincides with \( A_0 \). Then assuming that \( T_V \) and \( D_0^A \) overlap, we obtain, for some \( f^\perp \perp N_i, \nu \in N_i \)

\[
\frac{1}{A-iI} f^\perp = \nu - V \nu.
\]

Applying \( A_V - iI \) to both parts of this equation, we obtain

\[
f^\perp = -2i \nu,
\]

hence \( f^\perp = -2i \nu = 0 \).

*End of the proof.*
It follows from the Lemma that, once the extension is constructed on the Lagrangian plane, the whole construction of the extended operator can be accomplished in the form of a direct sum of the closure of the restricted operator and the extended operator on the Lagrangian plane. 

Note that the operator extension procedure may be developed without assumption of non-overlapping, see [34]. In particular, the case \( \dim E_A = 1 \), which is not formally covered by the above procedure, was analyzed in [70] independently of [34]. The relevant formulae for the scattering matrix and scattered waves remain true and may be verified by the direct calculation. We will use this fact in section 7 below.

We will use hereafter notations and some facts concerning the symplectic operator extension procedure, see Appendix and references therein. Choose an orthonormal basis in \( \mathcal{N} \):

\[
\{ f_s \}, \quad s = 1, 2, \ldots, d,
\]

as a set of deficiency vectors of the restricted operator \( A_0 \). Then the vectors \( \hat{f}_s = \frac{1}{A + iI} f_s \) form an orthonormal basis in the dual deficiency subspace \( N_{-i} \). Under the above non-overlapping condition one can use the formal adjoint operator \( A_0^+ \) defined on the defect \( N_i + N_{-i} = \mathcal{N} \):

\[
u = \sum_{s=1}^{d} [x_s f_s + \hat{x}_s \hat{f}_s] \in \mathcal{N}, \quad (75)
\]

by the von Neumann formula, see [3],

\[
A_0^+ u = \sum_{s=1}^{d} [-i x_s f_s + i \hat{x}_s \hat{f}_s]. \quad (76)
\]

In order to use the symplectic version of the operator-extension techniques we introduce in the defect a new basis \( W^\pm_s \), on which the formal adjoint \( A_0^+ \) is correctly defined due to the above non-overlapping condition:

\[
W^+_s = \frac{f_s + \hat{f}_s}{2}, \quad W^-_s = \frac{f_s - \hat{f}_s}{2i} = -\frac{I}{A - iI} f_s,
\]

\[
A_0^+ W^+_s = W^-_s, \quad A_0^+ W^-_s = -W^+_s.
\]

It is convenient to represent elements \( u \in \mathcal{N} \) via the new basis as

\[
u = \sum_{s=1}^{d} [\xi^+_s W^+_s + \xi^-_s W^-_s]. \quad (77)
\]

Then, using notations \( \sum_{s=1}^{d} \xi_{s, \pm} e_s := \xi_{\pm} \) we re-write the above von Neumann formula as

\[
u = \frac{A}{A - iI} \xi^+_+ - \frac{1}{A - iI} \xi^- - A_0^+ u = -\frac{1}{A - iI} \xi^- - A_0^+ u \quad (78)
\]

The following formula of integration by parts for abstract operators was proved in [53]:
Lemma 5.2. Consider the elements $u, v$ from the domain of the (formal) adjoint operator $A_0^+$:
\[
 u = \frac{A}{A - i\xi^+} - \frac{1}{A - i\xi^-}, \quad v = \frac{A}{A - i\xi^+} - \frac{1}{A - i\xi^-}
\]
with coordinates $\xi^\pm$:
\[
 \xi_i^\pm = \sum_{s=1}^d \xi_s^i f_{s,\pm} \in N_i, \quad \xi_i^\pm = \sum_{s=1}^d \xi_s^i f_{s,\pm} \in N_i.
\]
Then, the boundary form of the formal adjoint operator is equal to
\[
 J_A(u,v) = \langle A^+_0 u, v \rangle - \langle u, A^+_0 v \rangle = \langle \xi^+_+, \xi^-_+ \rangle - \langle \xi^-_-, \xi^+_+ \rangle.
\] (79)
One can see that the coordinates $\xi^\pm$ of the elements $u, v$ play the role of the boundary values $\{U'(0), U(0), V'(0), V(0)\}$. We will call them symplectic coordinates of the element $u, v$. The next statement proved in [53] is the core detail of the fundamental Krein formula [35], for generalized resolvents of symmetric operators. In our situation, it is used in course of calculation of the scattering matrix.

Lemma 5.3. The vector-valued function of the spectral parameter
\[
 u(\lambda) = \frac{A + i\lambda}{A - \lambda} \xi^+ := u_0 + \frac{A}{A - i\xi^-} - \frac{1}{A - i\xi^-}
\] (80)
satisfies the adjoint equation $[A_0^+ - \lambda I] u = 0$, and the symplectic coordinates $\xi^\pm$ of it are connected by the formula
\[
 \xi^-_+ = -P_{N_i} \frac{I + \lambda A}{A - \lambda} \xi^+_+
\] (81)
Proof: see in Appendix, subsection 9.1 or in [53].

Introduce the map
\[
 P_{N_i} \frac{I + \lambda A}{A - \lambda} P_{N_i} =: -M : N_i \to N_i.
\]
The matrix-function $M = P_{N_i} A P_{N_i} - P_{N_i} \frac{I + \lambda A}{A - \lambda} P_{N_i}$ has a negative imaginary part in the upper half-plane $\Im \lambda > 0$ and serves an abstract analog of the celebrated Weyl-Titchmarsh function. The operator-function $M$ exists almost everywhere on the real axis $\lambda$, and has a finite number of simple poles at the eigenvalues $\alpha^\pm$ of $A$. This function plays an important role in description of spectral properties of self-adjoint extensions of symmetric operators, see [35, 22].

We construct a solvable model of the quantum network as a self-adjoint extension of the orthogonal sum $l_o \oplus A_o$. We consider the orthogonal sum of the corresponding adjoint $l_o^+$ and the formal adjoint: $l_o^+ \oplus A_o^+$, and calculate the corresponding boundary form $J(U, V) := J(U, V) + J(u, v)$ on elements $(U, u) := U$ from the orthogonal sum of the corresponding spaces. The self-adjoint extensions of the operator $l_o \oplus A_o$ are obtained, based on restrictions of the adjoint operator $A_o^+ = l_o^+ \oplus A_o^+$ onto Lagrangian planes of the form $J(U, V)$. These planes may be defined by
the boundary conditions connecting symplectic coordinates \( U'(0), U(0), \vec{\xi}^+, \vec{\xi}^- \) of components of corresponding elements in the deficiency subspaces. For instance, one may select a finite-dimensional operator \( \beta : E_+ \oplus N_i \to E_+ \oplus N_i \) and define the Lagrangian plane \( L_{\beta} \) by the boundary condition

\[
\begin{pmatrix}
U'(0) \\
\vec{\xi}^+
\end{pmatrix}
= \begin{pmatrix}
\beta_{00} & \beta_{01} \\
\beta_{10} & 0
\end{pmatrix}
\begin{pmatrix}
U(0) \\
\vec{\xi}^-
\end{pmatrix}.
\] (82)

The extension defined by (82) on the Lagrangian plane is continued onto the whole space \( L_2(E_+, R_+ \oplus E_{\Lambda}) \) by forming the direct sum with the closure of the restricted operator \( A_0 \), see [34]. This construction gives a self-adjoint extension \( A_{\beta} \) of \( l_0 \oplus A_0 \) in \( L_2(E_+, R_+ \oplus E_{\Lambda}) \), defined by the boundary condition (82).

The absolutely continuous spectrum of the operator \( A_{\beta} \) coincides with the spectrum of the exterior part of the model, and hence it coincides with the spectrum of the trivial component \( l_{\Lambda} \) of the split operator \( L_{\Lambda} \) (in the open channels). The corresponding eigenfunctions of \( A_{\beta} \) on the first spectral band \( \Delta_1 \supset \Lambda \) can be found, see [4], via substitution into the above boundary condition for the column, combined of the Scattering Ansatz in the open channels with (80), and, in the outer space, with \( K_+ = \sqrt{\lambda - V \delta} + \pi^2 \delta^{-2} \):

\[
\Psi = \left( e^{iK_+ x} + e^{-iK_+ x} \right)
\] (83)

with \( \beta_{10} = \beta_{01}^+ \). It gives the linear equation for the Scattering Matrix:

\[
\left( iK_+ (\nu - S \nu) \right) = \begin{pmatrix}
\beta_{00} & \beta_{01} \\
\beta_{10} & 0
\end{pmatrix}
\begin{pmatrix}
\nu + S \nu \\
M \vec{\xi}^+
\end{pmatrix}.
\]

Solving this equation we obtain the scattered waves and the scattering matrix:

**Lemma 5.4.** The scattering matrix for the constructed extension is an analytic function of the spectral parameter \( \lambda \):

\[
S(\lambda) = \frac{iK_+ - [\beta_{00} + \beta_{01} M \beta_{10}]}{iK_+ + [\beta_{00} + \beta_{01} M \beta_{10}]},
\] (84)

with the denominator of the fraction preceding the numerator. The coordinate \( \vec{\xi}^+ \) of the inner component of the scattered wave (83) is defined as

\[
\vec{\xi}^+ = \beta_{10} \frac{2ip}{ip + [\beta_{00} + \beta_{01} M \beta_{10}]},
\]

with \( p = \sqrt{\lambda - V \delta + \pi^2 \delta^{-2}} \).

6. Fitting of the solvable model

It remains to choose the eigenvalues of \( A \), the subspace \( N_i \) and the matrix parameter \( \beta \), such that the operator-function \( [\beta_{00} + \beta_{01} M \beta_{10}] \) acting in \( E_+ \) coincides with the essential DN-map \( DN_{\Delta} \) of the intermediate Hamiltonian. Denote by \( Q_s \)
the spectral projection corresponding to the eigenvalue \( k^2 \) of \( A \), framed by the projections \( P_i \) onto the deficiency subspace \( N_i \),

\[ Q_s = P_i P_s. \]

Then the above expression takes the form:

\[
[\beta_{00} + \beta_{01}, M_{10}] = \\
\begin{bmatrix}
\beta_{00} + \sum_{r=1}^{N} \alpha^2 \alpha Q_s \beta_{10}
\end{bmatrix} - \sum_{r=1}^{N} \frac{1 + \alpha^4}{\alpha^2 - \lambda} \beta_{00} Q_s \beta_{10}.
\] (85)

We will define the boundary parameters \( \beta_{10}, \beta_{01} = \beta_{01}^* \) later, but once they are defined, we choose \( \beta_{00} \) such that the first summand in the right side of (85) coincides with \( k M \beta_{00} + \sum_{r=1}^{N} \alpha^2 \beta_{01} Q_s \beta_{10} = -k_M \). Then the scattering matrix takes the form:

\[
S(k) = \frac{i K + k_M + \sum_{r=1}^{N} \frac{1 + \alpha^4}{\alpha^2 - \lambda} \beta_{01} Q_s \beta_{10}}{i K + k_M - \sum_{r=1}^{N} \frac{1 + \alpha^4}{\alpha^2 - \lambda} \beta_{01} Q_s \beta_{10}},
\] (86)

which coincides with the essential scattering matrix if and only if the corresponding Krein function

\[
k_M - \sum_{r=1}^{N} \frac{1 + \alpha^4}{\alpha^2 - \lambda} \beta_{01} Q_s \beta_{10}
\] (87)

coincides with the essential part \( DN^{A}\lambda \) of the DN-map of the Intermediate Hamiltonian on the essential spectral interval \( \Delta \):

\[
DN^{A}\lambda \approx k(\lambda) + \sum_{r=1}^{N} \frac{P_+ \partial \varphi_r}{\nu_r}(P_+ \partial \varphi_r) + \lambda_r - \lambda.
\] (88)

Summarizing these results we obtain the following conditional statement for the extension constructed based on the boundary condition (82) in case when \( N_i \cap N_{-i} = 0 \) or \( \dim E_A = 1 \):

**Theorem 6.1.** The constructed operator \( A_{\beta_0} \) is a solvable model of the Quantum network on the essential interval \( \Delta \), if and only if the dimension of the space \( E_A \) coincides with the number \( N \) of eigenvalues of the intermediate operator on \( \Delta \subset [\lambda_{\text{max}}, \lambda_{\text{min}}] \), the eigenvalues \( \alpha_r^2 \) of the inner Hamiltonian \( A = \sum_{r=1}^{N} \alpha_r^2 \nu_r \) coincide with eigenvalues of the intermediate operator on \( \Delta \), there exists a deficiency subspace \( N_i \) of the inner Hamiltonian such that \( N_i \cap \frac{A_{\beta}}{A_{\beta_{01}}} N_i = 0 \) and the operator \( \beta_{01} : N_i \rightarrow E_+ \) such that for the orthonormal basis \( \{e_r\}_{r=1}^{N} \) of eigenvectors of \( A \) in \( E_A \)

\[
P_+ \frac{\partial \Psi_r}{\partial n} = [1 + \alpha_r^2]^{1/2} \beta_{01} P \nu_r, \quad r = 1, 2, \ldots, N.
\] (89)
Eliminating the inner variables, we can reduce the model to the Schrödinger equation with the constant potential on open channels, and appropriate boundary conditions on the bottom sections:

$$\frac{dU_\omega}{dx} |_{\Gamma} = \left[ k_M - \sum_{r=1}^{N} P_+ \frac{\partial \psi_r}{\partial n} \right] \left( \frac{\partial \Psi}{\partial n} \right) |_{\Gamma}.$$  \hspace{1cm} (90)

Unfortunately, this straightforward construction does not fulfill basic requirements of quantum mechanics, and hence we proceed via construction a self-adjoint operator in $[L_2(0, \infty) \times E_+] \oplus E_A$.

Dr. M. Harmer suggested an important strengthening of the previous conditional statement, by proving a general theorem of existence of the subspace $N_\Delta$ and the projection $P_{N_\Delta}$ which satisfy the condition of Theorem 4.1. The proof we provide below only slightly differs from the original proof in [26]: we added an explicit formula for $\beta_{01}$, $P_{N_\Delta}$ in terms of the corresponding Gram matrix.

Denote by $L_\Delta$ the restriction of the intermediate operator $L_\Lambda$ onto the invariant subspace $E_\Delta = E_A$ corresponding to the part $\sigma_\Delta = \{\lambda_1, \lambda_2, \ldots \lambda_N\}$ of its spectrum on the essential interval $\Delta$, and consider the linear map

$$\sum_s \left[ 1 + \alpha_s \right]^{-1/2} P_+ \frac{\partial \varphi_s}{\partial n} |_{\Gamma} \langle \cdot, \varphi_s \rangle := \Phi_\Delta$$

from $E_\Delta$ to $E_+, \dim E_+ = n$.

**Theorem 6.2. (M. Harmer)** The map $\Phi_\Delta$ defines a one-to-one correspondence between two $d$-dimensional subspaces, $2d < N$:

$$\Phi_\Delta^+ \Phi_\Delta E_\Delta := N_\Delta \subset E_\Delta$$

and

$$\Phi_\Delta \Phi_\Delta^+ E_+ := E_+ \subset E_+$$

If the subspace $N_\Delta$ is a generating subspace of $L_\Delta$ and

$$N_\Delta \cap \left( L_\Delta^* - iI \right)^{-1} \left( L_\Delta^* + iI \right) N_\Delta = 0,$$

then there exist a unique pair of the boundary operator $\beta_{01} : E_A \to E_+$ and the subspace $N_i \subset E_A$, which satisfy the condition of the previous theorem.

**Remark 2** This theorem gives an interpretation of the solvable model described in theorem 4.1, in terms of the intermediate Hamiltonian via selection of the inner Hamiltonian $A$ as a part $L_\Delta$ of $L_\Lambda$ in the invariant subspace corresponding to the essential spectral interval $\Delta$. The subspace $N_\Delta \subset E_\Delta$ plays the role of the deficiency subspace $N_i$ of the inner Hamiltonian and $\left( L_\Delta^* - iI \right)^{-1} \left( L_\Delta^* + iI \right) N_\Delta$ plays the role of the dual subspace $N_{-i}$.  

**Proof** The map $\Phi_\Delta$ is represented by the $n \times N$ matrix $\Phi$ of columns $\phi_s$ with respect to the orthogonal basis of cse-functions $\{e_s\}$ in $E_+$. The condition (89) is equivalent to the representation of the operator $\Phi_\Delta$ in form $\beta_{01} P_{N_\Delta}$, where $\beta_{01}$ is a bounded operator acting from $E_A$ into $E_+$ and $P_{N_\Delta}$ is an orthogonal projection.
in $E_\Lambda$ onto the deficiency subspace $N_i$. We will construct both $\beta_{01}$, $P_{N_i}$ from the data encoded in $\Phi_\Lambda$.

The non-negative Gram operator $\Phi_\Lambda \Phi_\Lambda^+$ in $E_\Lambda$ has the spectral representation

$$\Phi_\Lambda \Phi_\Lambda^+ = U^+ D U.$$  

The non-negative diagonal matrix $D$ is invertible on the orthogonal complement $\hat{E}$ of the corresponding null-space $\hat{E}_0$. We denote the restriction $D$ onto $\hat{E}$ by $\hat{D}$. One can assume that the subspace $\hat{E}$ belongs to some extended space $\hat{E} \oplus \hat{E}_0$ which contains $E_\Lambda$, and the operator $U^+$ acts from $\hat{E} \oplus \hat{E}_0$ onto $E_\Lambda$ as an isometry.

The operator $U^+ \hat{D}^{1/2}$ coincides with $\Phi_\Lambda$. Hence the operator $\Phi_\Lambda$ is presented as a product $\beta \hat{P}$, with $\beta = \beta_{01} = U^+ \hat{D}^{1/2} : \hat{E} \to E_\Lambda$ and $\hat{P} = P_{\hat{E}} := P_{N_i} \subset E_\Lambda$, $\dim N_i = \dim \hat{E} = d$ and coincides with the dimension of the resonance entrance subspace of the intermediate operator. Up to some non-essential isometry we may assume that $E_\Lambda = E_\Lambda, A = L_\Lambda, N_i = N_\Lambda$. The condition (92) guarantees that $N_i \cup N_{-i} = 0$.

End of the proof

In the case when only one resonance eigenvalue $\alpha_2$ of the intermediate operator sits on the essential spectral band, the obtained model scattering matrix

$$S(p) = \frac{iK_+ - k_M + \frac{1+\alpha_4}{\alpha_0 - \lambda} \beta_{01} Q_0 \beta_{10}}{iK_+ + k_M - \frac{1+\alpha_4}{\alpha_0 - \lambda} \beta_{01} Q_0 \beta_{10}}$$

is a single-pole approximation of the scattering matrix of the network. The condition of the above theorem is obviously fulfilled for the single-pole approximation, when $P \frac{\partial \varphi_0}{\partial n} \neq 0, d = 1, N = 1,$ and $\beta_0$ is a one-dimensional operator mapping the one-dimensional subspace $N_i$ onto the resonance entrance subspace in $E_\Lambda$ spanned by $P \frac{\partial \varphi_0}{\partial n}$. For thin or shrinking networks one can estimate, (see [6] and more details in [42, 43]) the deviation of the single-pole and/or few-poles approximations from the exact scattering matrix on the network, in terms of the ratio $d/$diam $\Omega_{in}$. We postpone the discussion of the non-stationary scattering matrix for QN to forthcoming publications. But we notice here that the local wave operators (see [8]) and the corresponding scattering matrix on the essential spectral band can be defined for the pair $(\mathcal{L}, A_\delta)$.

7. A solvable model as a jump-start in the analytic perturbation procedure

Recall that the exact scattering matrix was approximated by the essential or approximate scattering matrix. In this section we consider this phenomenon from
the point of view of complex analysis, for the simplest star-shaped network constructed of a single model quantum well with one semi-infinite wire attached to it.

Consider a thin quantum network constructed of a quantum well $\Omega$ and a single quantum wire of width $\delta$ attached to it, $\delta/diam\Omega \ll 1$. Assume that the Fermi level is situated on the first spectral band in the wire, which has multiplicity 1. Without loss of generality we may assume that the component of the corresponding solvable model in the open channel is presented by the Schrödinger equation with

$$2\mu^\parallel = 2\mu^\perp = I, \ V^\circ = V, \ K^\perp = p = \sqrt{\lambda - \frac{\pi^2}{\delta^2} - V}$$

and one-dimensional subspace $E^+$:

$$-u'' = p^2 u, \ 0 < x < \infty.$$  \hspace{1cm} (94)

Assume that the model Hamiltonian $A_\beta$ is constructed as suggested in the previous section based on the “inner Hamiltonian” $A$, the differential operator $l_\lambda$ and the boundary parameters which are reduced to the coupling constant $\beta_{01} := \beta$. Hereafter we will use the re-normalized eigenvalues $\alpha^2 - \frac{\pi^2}{\delta^2} - V := k_s^2 > 0$. Introducing that notation into the Krein function, and submitting the boundary parameter to the condition $\beta_{00} + \sum_{s=1}^N \alpha_s^2 \beta_{s0} q_s \beta_{1s} = 0$ we obtain the corresponding few-pole scattering matrix as a function of the wave-number $p$, with physically meaningful limit behavior at infinity $S_\beta(p) \to I$:

$$S_\beta(p) = \frac{ip - k - \beta^2 \sum_{s \neq 0} \frac{1 + \alpha_s^4}{p^2 - k_s^2} q_s}{ip + k + \beta^2 \sum_{s \neq 0} \frac{1 + \alpha_s^4}{p^2 - k_s^2} q_s}.$$  \hspace{1cm} (95)

Here $q_s = |\langle e, e_s \rangle|^2$. Zeros $p_\beta(\beta)$ of the Scattering matrix (94) - the resonances - sit in the upper half-plane $\Im p > 0$ and approach the points $\pm k_s, \ k_{s-} := -k_s$, when $\beta \to 0$.

Assume that the resonance eigenvalue $\alpha_{00}^2 = k_0^2 + \delta^2 \pi^2 + V$ is situated close to the scaled Fermi-level $\Lambda$ and the coupling constant $\beta := \beta_{01}$ is relatively small, see below. Separating the resonance term in the numerator and denominator of (95)

$$\left[ ip - \beta^2 \frac{1 + \alpha_0^4}{k_0^2 - p^2} q_0 \right] + \left[ k + \beta^2 \sum_{s \neq 0} \frac{1 + \alpha_s^4}{p^2 - k_s^2} q_s \right],$$

and multiplying by $(ip)^{-1}$ one can see that $\frac{-\beta^2}{ip} \left[ k + \sum_{s \neq 0} \frac{1 + \alpha_s^4}{p^2 - k_s^2} q_s \right]$ plays the role of the small parameter. The resonance $k_\beta(\beta)$ originated from the eigenvalue $k_0^2$ of the operator $A$ (more precisely : from the point $+k_0$) can be obtained as a solution $p = k_\beta(\beta)$ of the equation

$$p = k_0 - \frac{\beta^2 (1 + \alpha_0^4)q_0}{(p + k_0)} \left( ip + k + \beta^2 \sum_{s \neq 0} \frac{1 + \alpha_s^4}{p^2 - k_s^2} q_s \right).$$  \hspace{1cm} (96)
Another resonance originated from the point \(-k_0\) corresponds to the same eigenvalue, and it sits at the symmetric point \(-\bar{k}_0(\beta)\) with respect to the imaginary axis. Remaining resonances \(k_s(\beta)\), \(s \neq 0\), can be found from similar equations. All functions \(k_s(\beta)\) are analytic functions of \(\beta, k\) in small neighborhoods of \((0, \pm k_0)\). They sit in the upper half-plane symmetrically with respect to the imaginary axis \(k_s(\beta) = -\bar{k}_s(\beta)\). The scattering matrix \((95)\) is unitary on the real axis \(k\) and has poles at the complex-conjugate points \(\bar{k}_s(\beta)\) in the lower half-plane, and hence it is presented by the finite Blaschke product which tends to 1 when \(|k| \to \infty\):

\[
S^\beta(p) = \prod_s \frac{p - k_s(\beta)}{p - k_s(\beta)}.
\] (97)

The outer component of the scattered wave is presented as

\[
\Psi^\beta_0 = e^{-ipx} + S^\beta(k)e^{ipx}.
\] (98)

It fulfills appropriate boundary condition at the place of contact with the model quantum dot. The inner component of the scattered wave can be obtained from Lemma 3.4.

We explore the model scattering problem for small values of \(\beta\). Though the resonances depend analytically on \(\beta\), neither the scattering matrix \((95, 97)\) nor the scattered wave depend analytically of \((\beta, p)\) on the product of a small neighborhood of the origin in \(\beta\)-plane and small neighborhoods of \(\pm k_0\) in \(p\)-plane. The analyticity is lost due to presence of the points \(\pm k_0\) where the resonances are created at \(\beta = 0\): both \(k_0(\beta)\) and \(\bar{k}_0(\beta)\) approach the same point \(k_0\) when \(\beta \to 0\).

The corresponding “resonance” factor of the scattering matrix

\[
S^\beta_0(p) = \left[ \frac{p - k_0(\beta)}{p - k_0(\beta)} \right] \left[ \frac{p + \bar{k}_0(\beta)}{p + \bar{k}_0(\beta)} \right],
\] (99)

is non-analytic on \((\Omega_\beta \times \Omega_{k_0} \times \Omega_{-k_0})\), though \(k_\beta = \Re k_\beta + i\Im k_\beta\) is analytic function of \(\beta\) due to \((96)\). But the complementary factor of the scattering matrix

\[
S^\beta_- (p) = \prod_{s \neq 0} \frac{p - k_s(\beta)}{p - k_s(\beta)}.
\] (100)

is analytic on \((\Omega_\beta \times \Omega_{k_0} \times \Omega_{-k_0})\) and can be expanded into the power series over \(\beta^m, m = 0, 1, 2, \ldots\). Assume now that the function \(k_\alpha(\beta)\) is known. Then the following statement is true:

**Theorem 7.1.** There exists a one-dimensional perturbation \(A_0^\alpha\) of the operator

\[
l_0u = -u'', \quad u\bigg|_a = 0
\]

with a non-trivial inner component, such that the scattering matrix of the pair \((A_0^\alpha, l_0)\) coincides with \(-S^\alpha_0(p)\). Then the scattering matrix \(S\) of the complementary
pair \((A_\beta, A_0^\beta)\) is equal to the complementary factor \(-S_\beta^0(p)\):

\[
S_\beta(p) = S_\beta^0(p) S_\beta^0(p).
\]

The complementary factor is an analytic function of \((\beta, k)\) on the product \((\Omega_\beta \times \Omega_{k_0} \times \Omega_{-k_0})\) of a small neighborhood of the origin in \(\beta\)-plane and a small neighborhood of the pair \((k_0, -k_0)\) in the \(p\)-plane.

**Proof** is presented in [59].

**Corollary 1** The exterior component of the scattered wave of the operator \(A_\beta^a\) presented by the Ansatz (98) with \(S_\beta\) taken in the form (97) is not analytic with respect to the coupling constant \(\beta_01 := \beta\) near the origin. The non-analyticity of the scattered wave is caused by the presence of the non-analytic factor \(-S_0^a\) in the scattering matrix. From theorem 4.1, we interpret this factor as the scattering matrix for the pair \(\left(A_\beta^a, l_o\right)\). The complementary factor \(-S_\beta^0\) is analytic with respect to the coupling constant \(\beta\). It can be interpreted as the scattering matrix for the pair \(\left(A_\beta^a, A_0^\beta\right)\). Summarizing our observation we suggest, for our example, the following two-steps modification of the analytic perturbation procedure on continuous spectrum:

a. First step is the construction of the solvable model and calculation of the corresponding (non-analytic with respect to the coupling constant \(\beta_0 := \beta\)) scattering matrix. This is “the jump-start” of the analytic perturbation procedure.

b. Second step is the calculation of the analytic factor of the scattering matrix of the model by the standard analytic perturbation procedure. The analytic factor is interpreted as the scattering matrix between the constructed solvable model and the perturbed operator \(A_\beta^a\).

The obtained connection between resonances and analytic perturbation series on the continuous spectrum recalls the connection between small denominators in celestial mechanics and divergence of perturbation series, observed by H. Poincaré, see [62]. More historical comments about intermediate Hamiltonian and the jump-start may be found in [55], where similar modification of the analytic perturbation procedure for the Friedrichs model is suggested.

**Remark 3** Note that recovering exact information on the resonance \(k_0(\beta)\) and on the corresponding residue for the perturbed operator \(A_\beta^a\), which we need to develop the “jump-start” procedure, may be a tricky problem almost equivalent to the original spectral problem. On the other hand, if the approximate resonance factor \(S_0^a\) is used instead of the exact factor, then the division of the scattering matrix through \(S_0^a\) would not eliminate singularity, hence the complementary factor of the scattering matrix would be still non-analytic at the origin and hence could not be obtained via analytic perturbation procedure.
8. Acknowledgement

The author acknowledges support from the Russian Academy of Sciences, Grant RFBR 03-01-00090. The author is grateful to V. Katsnelson for important references and very interesting materials provided, and to M. Harmer for deep remarks concerning the fitting of the star-graph model.

9. Appendix: symplectic operator extension procedure

John von Neumann in 1933 has found conditions which guarantee existence of a self-adjoint extension of given unbounded symmetric operator, and suggested a procedure of construction of the extension, see symplectic version in [53]. For given symmetric operator \( A_0 \) defined on \( D_0 \) in the Hilbert space \( H \), see [3] and given complex value \( \lambda, \Im \lambda \neq 0 \) of the spectral parameter:

**Definition 9.1.** Define the deficiency subspaces

\[
N_\lambda := H \ominus [A_0 - \lambda I]D_0, \\
N_{\bar{\lambda}} := H \ominus [A_0 - \bar{\lambda} I]D_0.
\]

The dimension of \( N_\lambda, N_{\bar{\lambda}} \) is constant on the whole upper and lower spectral half-plane \( \Im \lambda > 0, \Im \lambda < 0 \) respectively.

**Definition 9.2.** Introduce the deficiency index \((\dim N_\lambda, \dim N_{\bar{\lambda}}) := (n_+, n_-)\) of the operator \( A_0 \).

J. von Neumann proved that

**Theorem 9.1.** The hermitian operator \( A_0 \) has a self-adjoint extension if and only if \( n_+ = n_- \).

The idea of construction of the extension is based on the following theorems von Neumann, see for instance [3]:

**Theorem 9.2.** The domain of the adjoint operator is represented as a direct sum of the closure and the deficiency subspaces, in particular:

\[
D_{A_0^*} = D_{\bar{A}_0} + N_i + N_{-i}.
\]

The deficiency subspaces of the densely-defined operator are the eigen-spaces of the adjoint operator:

\[
A_0^*e_i = -ie_i, \quad e_i \in N_i, \quad A_0^*e_{-i} = ie_{-i}, \quad e_{-i} \in N_{-i}.
\]

**Theorem 9.3.** If \( A_0 \) is an Hermitian operator with deficiency indices \((n_+, n_-)\), \( n_- = n_+ \) and \( V \) is an isometry \( V : N_i \to N_{-i} \). Then the isometry \( V \) defines a self-adjoint extension \( A_V^* \) of \( A_0 \), acting on the domain

\[
D_{A_V} = D_{\bar{A}_0} + \{e_i + Ve_i, \quad e_i \in N_i\}
\]

as a restriction of \( A_0^* \) onto \( D_{A_V} \):

\[
A_V : u_0 + e_i + Ve_i \to \bar{A}_0u_0 - ie_i + iVe_i.
\]
J. von Neumann reduced the construction of the extension of the symmetric operator $A_0$ to an equivalent problem of construction of an extension of the corresponding isometrical operator - the Caley transform of $A_0$. It is much more convenient, for differential operators, to construct the extensions based on so-called boundary form.

**Example 5. Symplectic Extension procedure for the differential operator** Consider the second order differential operator

$$L_0 u = - \frac{d^2 u}{dx^2},$$

defined on all square integrable functions, $u \in L_2(0, \infty)$, with square-integrable derivatives of the first and second order and vanishing near the origin. This operator is symmetric and its adjoint $L_0^+$ is defined by the same differential expression on all square integrable functions with square integrable derivatives of the first and second order and no boundary condition at the origin. This operator is not symmetric: its boundary form $J(u, v) = \langle L_0^+ u, v \rangle - \langle u, L_0^+ v \rangle = u'(0)\bar{v}(0) - u(0)\bar{v}'(0)$, $u, v \in D_{L_0^+}$, is generally non-equal to zero for $u, v \in D_{L_0^+}$. But it vanishes on a "Lagrangian plane" $P_\gamma \subset D_{L_0^+}$ defined by the boundary condition $u'(0) = \gamma u(0), \gamma = \bar{\gamma}$.

The restriction $L_\gamma$ of the $L_0^+$ onto the Lagrangian plane $P_\gamma$ is a self-adjoint operator in $L_2(0, \infty)$: it is symmetric, and the inverse of it ($L_\gamma - \lambda I$)$^{-1}$, at each complex spectral point $\lambda$, exists and is defined on the whole space $L_2(0, \infty)$.

The operator extension procedure used above for the differential operator, can be applied to general symmetric operators and serves a convenient alternative for construction of solvable models of orthogonal sums of differential operators and finite matrices. We call the abstract analog of the extension procedure the symplectic extension procedure. Let $A$ be a self-adjoint operator in a finite-dimensional Hilbert space $E$, $\dim E = d$, and $N_i := N$ is a subspace of $E$, $\dim N = n < d/2$, which does not overlap with $\frac{A + iI}{A - iI}N_i := N_{-i}$:

$$N_i \cap N_{-i} = \{0\}.$$  

Define the operator $A_0$ as a restriction of $A$ onto $D_0 := \frac{L}{A - iI}E \ominus N$. This operator is symmetric, and the subspaces $N_{\pm i}$ play roles of it’s deficiency subspaces. The operator can $A_0$ can be extended to the self-adjoint operator $A_0^+ \supset A_0$ via symplectic extension procedure involving the corresponding boundary form: selecting a basis $\{e^+\}_{s=1}^n := g_s \in N_i$, we consider the dual basis $\left\{ \frac{A + iI}{A - iI}g_s = g_s^- \right\}_{s=1}^n \in N_i$. Introduce, following [53], another basis in the defect $N = N_i + N_{-i}$

$$W^+ := \frac{1}{2} \left[ g_s + \frac{A + iI}{A - iI}g_s \right], \quad W^- := \frac{1}{2i} \left[ s - \frac{A + iI}{A - iI}g_s \right].$$

Due to $A_0^+ g_s + ig_s = 0$, $[A_0^+ - iI]A_{N_i} g_s = 0$ we have,
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\[ A^+_0 W^+_s = W^-_s, \quad A^+_0 W^-_s = -W^+_s. \]

Following [24] we will use the representation of elements from the domain of the adjoint operator by the expansion on the new basis:

\[ u = u_0 + \sum_s \xi^+_s W^+_s + \xi^-_s W^-_s, \]

with \( u_0 \in D(A_0) \) and simplectic coordinates \( \xi^\pm_s \).

We also introduce the boundary vectors of elements from \( D(A^+_0) \)

\[ \tilde{\xi}^\pm := \sum_s \xi^\pm_s g_s \in N_i, \]

\[ u = u_0 + \frac{A}{A - iI} \tilde{\xi}^u_+ - \frac{I}{A - iI} \tilde{\xi}^u_- := u_0 + n^u, \quad u_0 \in D(A_0) n^u \in N. \]

Define the formal adjoint operator \( A^+_0 \) on the defect \( N = N_i + N_{-i} \) as:

\[ A^+_0 e_+ = -i e_+, \quad \text{for} \quad e_+ \in N_i, \quad A^+_0 e_- = i e_-, \quad \text{for} \quad e_- \in N_{-i}, \]

\[ A^+_0 (e_+ + e_-) = -i e_+ + i e_. \]

Then we have:

\[ A^+_0 W^+_s = W^-_s, \quad A^+_0 W^-_s = -W^+_s. \]

Following [53], we will use the representation of elements from the domain of the adjoint operator by the expansion on the new basis:

\[ u = u_0 + \sum_s \xi^+_s W^+_s + \xi^-_s W^-_s, \]

with \( u_0 \in D(A_0) \) and simplectic coordinates \( \xi^\pm_s \). We also introduce the boundary vectors of elements from \( D(A^+_0) \)

\[ \tilde{\xi}^\pm := \sum_s \xi^\pm_s g_s \in N_i, \]

\[ u = u_0 + \frac{A}{A - iI} \tilde{\xi}^u_+ - \frac{I}{A - iI} \tilde{\xi}^u_- := u_0 + n^u, \quad u_0 \in D(A_0) n^u \in N. \]

Then the boundary form of \( A^+_0 \) is calculated as

\[ \langle A^+_0 u, v \rangle - \langle u, A^+_0 v \rangle := \mathcal{J}(u, v) = \langle \tilde{\xi}^u_+, \tilde{\xi}^v_+ \rangle - \langle \tilde{\xi}^u_-, \tilde{\xi}^v_- \rangle. \]
9.1. Operator Extensions: Krein formula

**Theorem: Krein formula** Consider a closed symmetric operator $A_0$ in the Hilbert space $H$, obtained via restriction of the self-adjoint operator $A$ onto the dense domain $D(A_0)$, with finite-dimensional deficiency subspaces $N_{\mp i}$, $P_{N_i} := P_\mp$, $\dim N_i = \dim N_{-i}$. Then the resolvent of the selfadjoint extension $A_M$ defined by the boundary conditions

$$\xi_+ = M\xi_-$$

is represented, at regular points of $A_M$, by the formula:

$$(A_M - \lambda I)^{-1} = \frac{I}{A - \lambda I} - \frac{A + iI}{A - \lambda I} P_+ M \frac{I + P_+ \frac{A - iI}{A - \lambda I} P_+ M}{I + P_+ \frac{A - iI}{A - \lambda I} P_+ M} P_+ \frac{A - iI}{A - \lambda I}$$

**Proof.** For the convenience of the reader we provide below the sketch of the proof of the Krein formula via simplectic operator extension procedure. Solution of the homogeneous equation $(A^+ - \lambda I) u = f$ is reduced to finding $u_0, \xi_\pm$ from the equation

$$(A - \lambda I) u_0 - \frac{I + \lambda A}{A - iI} \xi_+ - \frac{A - \lambda I}{A - iI} \xi_- = f.$$  

(102)

Applying to this expression the operator $\frac{A - iI}{A - \lambda I}$, due to $(A - iI) u_0 \perp N_i$, we obtain

$$\xi_- = \frac{I}{I + \frac{A - iI}{A - \lambda I} P_+} A - \lambda I.$$  

Then, from the above equation (102) and from the boundary condition (101), we derive:

$$u_0 = \frac{1}{A - iI} \left[ I + \lambda A \xi_+ + \xi_- \right] + \frac{I}{A - \lambda I} f,$$

and

$$u = u_0 + \frac{A}{A - iI} \xi_+ - \frac{I}{A - \lambda I} \xi_- = \frac{I}{A - \lambda I} f - \frac{A + iI}{A - \lambda I} P_+ M \frac{I + P_+ \frac{A - iI}{A - \lambda I} P_+ M}{I + P_+ \frac{A - iI}{A - \lambda I} P_+ M} P_+ \frac{A - iI}{A - \lambda I} f.$$  

The end of the proof

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