

MODIFIED KREIN FORMULA AND ANALYTIC PERTURBATION PROCEDURE FOR SCATTERING ON ARBITRARY JUNCTION

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A quantum network is constructed of straight quantum wires- the leads, of constant width,- and quantum wells, which play roles of the vertex domains of the network. Basic element of the network is the junction: a detail of the network consisting of a single compact quantum well and few semi-infinite wires attached to it. In the theoretical study of the one-body transport on a junction, the role of the Hamiltonian is played by the one-body Schrödinger operator. In case when the corresponding potential is a real constant in the wires and is a piecewise continuous bounded real function on the quantum well, the transport problem is reduced to the one-body scattering problem.

In this paper we suggest a semi-analytic perturbation procedure which permits to calculate the one- body scattering parameters for arbitrary junction, based on a specially selected intrinsic large parameter. This procedure gives us an approximate scattering matrix. The suggested analytic perturbation procedure is applicable to any junction based on a compact vertex domain, with piece-wise smooth boundary. Scattering matrix of a thin junction is approximated by the scattering matrix of the corresponding solvable model.

1 Introduction

In this paper we denote by Ω_s the vertex domains (the quantum wells) and by ω^m the leads (quantum wires), of equal width δ connecting the wells to each other or extending to infinity. It is convenient to assume, that the domains and the leads are separated from each other by imaginable orthogonal bottom

sections γ_m , $\cup_m \gamma_m = \Gamma$, see Fig. 1 below. The dynamic of a single electron on the network $\Omega : \{\cup_s \Omega_s\} \cup \{\cup_m \omega^m\}$ is described by the Schrödinger equation which is transformed, after separation of time and scaling of energy $E \rightarrow \lambda = 2m_0 E \hbar^{-2}$, to the spectral problem for the Schrödinger operator \mathcal{L} on the network:

$$\mathcal{L}\psi = -\frac{1}{2\mu} (\nabla + A)^2 \psi + H_R \psi + V\psi = \lambda\psi, \quad (1)$$

where m_0 is the conventional electron mass, and $\mu = m^*/m_0$ is the ratio of the effective mass and the conventional mass. The magnetic potential A and the Rashba Hamiltonian, see [1] are continuous and vanish on the wires, the potential V is a real constant V_δ on the wires and it is a piecewise continuous function V_s on the quantum wells Ω_s . We consider hereafter a star shaped network - a *junction*- with a single well Ω_{int} (the inner part of the network), and few quantum wires ω^n attached to it. Hereafter we denote by $\omega := \cup_n \omega^n = \Omega \setminus \Omega_{int}$ the “exterior part” of the network.

Theoretical analysis of the electron transport problem in the junction is usually reduced to one-electron scattering problem, see [1-3], for the pair of Hamiltonians: the one electron Schrödinger operator \mathcal{L} on the whole junction Ω and the splitting of it $\mathcal{L} \rightarrow L_{int} \oplus l^\omega := \mathcal{L}_0$ which is an orthogonal sum of $L_{int} = \mathcal{L}|_{L_2(\Omega_{int})}$ and $l^\omega = \mathcal{L}|_{L_2(\omega)}$, obtained via imposing of additional zero boundary condition - a mathematical version of the “solid wall” - on Γ . The part

$$l^\omega := -2\mu^{-1} \Delta + V_\delta$$

of the split operator on the exterior part of the junction plays a role of a standard unperturbed Hamiltonian in the above scattering problem. This scattering problem is a sophisticated perturbation problem for the operator \mathcal{L}_0 which has embedded eigenvalues. Under the perturbation - removing the solid wall on Γ - the standing waves in the vertex domain Ω_{int} are bred with the running waves in the wires, resulting in resonances which define the resonance character of the transmission across the junction. Analytical calculation of the scattering matrix of the two-dimensional junction is a difficult mathematical problem concerning perturbation of embedded eigenvalues. For practical needs of mathematical design of quantum networks with prescribed transport properties physicists substitute the networks by quantum graphs, with an appropriate boundary condition at the vertices, see [3, 4, 5]. Validity of that solvable model was confirmed by smooth approximation of the graph by thin manifold shrinking to the graph, see for instance

[6, 7]. This analysis showed that, in particular, for uniform shrinking, the eigenvalues, *at the lower spectral threshold*, $\lambda = 0$ of the two-dimensional Laplace equation on the manifold - the “fattened graph”, with Neumann boundary conditions, - converge to the eigenvalues of the one-dimensional Schrödinger equation on the graph, with the Kirchhoff boundary condition at the vertex $a : \sum_s \frac{d\psi_s}{dx}(a) = 0$. This mathematical result is proved in [7], and remains valid for various spectral problems on fattened graphs, in particular, for the spectral problem of diffusion, where the spectral properties of the relevant second order partial differential operator near the threshold $\lambda = 0$ are important ¹

Contrary to diffusion, scattering of electrons in quantum networks is observed on the small, for low temperature, essential spectral interval centered at the Fermi level [9] which can be situated well above the lower threshold. In [10, 11] the *resonance mechanism* of conductance across the junction is considered. For thin junction the role of main detail of the transmitting mechanism is played by the resonance eigenfunction φ_0 , which corresponds to the eigenvalue λ_0 of the Schrödinger operator on the vertex domain, which is the closest to the scaled Fermi - level Λ^F . The magnitude of the transmission coefficient is defined by the shape of the resonance eigenfunction of the Schrödinger operator on the vertex domain of the junction. The resonance mechanism permits to interpret the phenomenological parameter in the boundary condition suggested by Datta ([2]) for T-junction.

In this paper we suggest a modified analytic perturbation procedure for calculation of the scattering matrix of *arbitrary junction*, on a given essential interval centered at the Fermi level and containing no spectral thresholds. For thin junction the role of the first step - “jump-start” - in this analytic perturbation procedure is played by the solvable model of the junction which is completely fitted based on spectral data of the Schrödinger operator on the vertex domain of the junction.

2 Scattering in Quantum Networks

Consider a junction Ω constructed of the vertex domain - a quantum well Ω_{int} - and the straight leads - quantum wires ω^m , of equal width δ connecting the well to the infinity, $\cup_m \omega^m := \omega$. It is convenient to assume, that the domain

¹Note that in [8] a violation of some version of Kirchhoff boundary condition is noticed for electrons on a quantum network.

[ht]

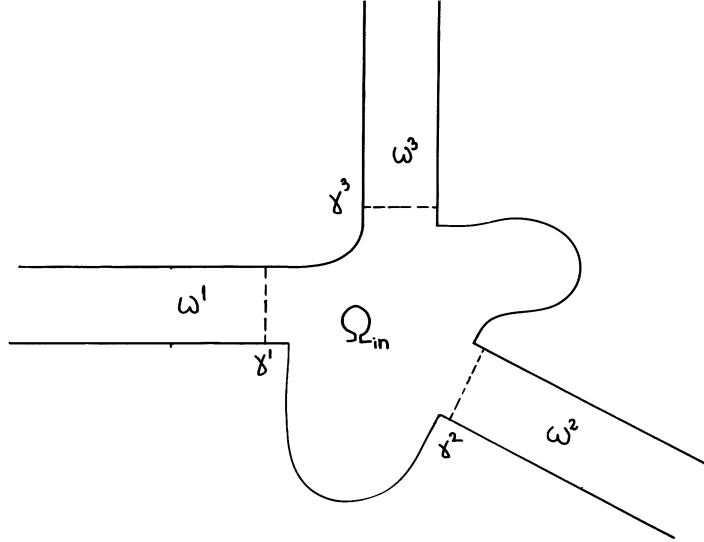


Figure 1: A junction.

Ω_{int} and the wires ω^m are separated from each other by imaginable orthogonal bottom sections γ^m , $\cup_m \gamma^m = \Gamma$, see (2).

The dynamic of a single electron on the network is governed by the Schrödinger equation which becomes equivalent, after separation of time and scaling of energy $E \rightarrow \lambda = 2m_0 E \hbar^{-2}$, to the spectral problem for the Schrödinger operator \mathcal{L} on Ω , see below (1).

The role of the wave function is played by the 2-spinor ψ . The spin-orbital interaction is defined by the symmetrized Rashba “Hamiltonian”:

$$H_R = \alpha(x)[\sigma, p] + [\sigma, p]\alpha(x), \quad p = i\nabla,$$

containing the Rashba - factor α , see [1], defined by the magnitude of the normal component of electric field. We assume that the factor vanishes near the boundary $\partial\Omega$ and on the wires. Hence the corresponding Schrödinger equation has the form (1). We assume that the temperature is low and the Fermi level $\Lambda^F = 2m_0 E_F \hbar^{-2}$ lies deep enough below the potential on the

complement $R_3 \setminus \Omega$, to assume that ψ vanishes on the boundary $\partial\Omega$ of the network. The above one-electron Hamiltonian \mathcal{L} is selfadjoint in the Hilbert space $L_2(\Omega_{int} \cup \omega)$ of all square-integrable functions. The transport properties of the junction are defined by the structure of the scattered waves - the eigenfunctions of continuous spectrum of \mathcal{L} . We consider also the Schrödinger equation $L_{int}\psi = \lambda\psi$, on the quantum well Ω_{int} with L_{int} defined by the same magnetic field, the potential and the Rashba term as \mathcal{L} , and additional zero boundary condition on Γ .

The one - body transport problem for the quantum network is solved on the spectral interval Δ if all scattered waves are constructed for the values of energy $\lambda \in \Delta$. For given temperature T an essential spectral interval $\Delta_T := \Delta$ is centered on the scaled Fermi level, see [9], $E^F \rightarrow \Lambda^F = 2m_0 E^F \hbar^{-2}$, as

$$\Delta = [\Lambda^F - 2m_0\kappa T \hbar^{-2}, \Lambda^F + 2m_0\kappa T \hbar^{-2}]. \quad (2)$$

Hereafter we assume that neither of spectral thresholds $\pi^2 l^2 \delta^{-2} + V_\delta$ is situated on the Δ . For given scaled Fermi level the spectral branches $\sigma_l := [\pi^2 l^2 \delta^{-2} + V_\delta, \infty)$ can be classified into two categories : open branches $[\pi^2 l^2 \delta^{-2}, \infty)$, corresponding to the lower group of thresholds

$$\pi^2 l^2 \delta^{-2} + V_\delta < \Lambda^F,$$

and closed branches, corresponding to the upper group of thresholds

$$\pi^2 l^2 \delta^{-2} + V_\delta > \Lambda^F.$$

These branches are characterized by the behavior of the corresponding exponential modes on the leads for $\lambda \in \Delta$

1. Oscillating modes:

$$\chi_\pm^l(x) := \exp\left(\pm i \sqrt{\lambda - V_\delta - \pi^2 l^2 \delta^{-2}} x^\parallel\right) e_l(x^\perp),$$

in open branches of the wires, $\lambda - V_\delta - \pi^2 l^2 \delta^{-2} > 0$, with cross-section eigenfunctions $e_l(x^\perp) = \sqrt{2/\delta} \sin \pi l x^\perp / \delta \vec{e}_l$, $l = 1, 2, \dots$, $0 < x^\parallel < \infty$, $0 < x^\perp < \delta$ for $x = (x^\perp, x^\parallel) \in \omega^m$, with a constant normalized 2-d spinors \vec{e}_l in each wire, and

2. Similar exponentially decreasing modes

$$\xi^l(x) := \exp\left(-\sqrt{\pi^2 l^2 \delta^{-2} + V_\delta - \lambda} x^\parallel\right) e_l(x^\perp),$$

in closed branches of the wires $\pi^2 l^2 \delta^{-2} + V_\delta - \lambda > 0$.

The above modes satisfy formally the differential equation :

$$\mathcal{L}\chi_\pm^l = \lambda\chi_\pm^l, \quad \mathcal{L}\xi^l(x) = \lambda\xi^l(x),$$

and vanish on both shores of the leads. The scattered waves are obtained via matching on $\Gamma := \{x : x^\parallel = 0\}$ of the solution of the Schrödinger equation $L_{int}\psi = \lambda\psi$ in Ω_{int} , $\psi \Big|_{\partial\Omega_{int}\setminus\Gamma} = 0$, to the scattering Ansatz $\vec{\psi}(x, \lambda) = \{\psi_l^m(x, \lambda)\}$ in the wires ω^m . The scattering Ansatz on the exterior part $\omega := \cup_m \omega^m$ of the network is combined of the exponential above modes as

$$\begin{aligned} \psi_l^m(x) = & \\ \left\{ \begin{array}{l} \chi_+^l(x) + \sum_{\pi^2 r^2 / \delta^2 < \lambda} S_{l,r}^{m,m} \chi_-^r(x) + \sum_{\pi^2 r^2 / \delta^2 > \lambda} s_{l,r}^{m,m} \xi^r(x), x \in \omega^m \\ \sum_{\pi^2 r^2 / \delta^2 < \lambda} S_{l,r}^{m,n} \chi_-^r(x) + \sum_{\pi^2 r^2 / \delta^2 > \lambda} s_{l,r}^{n,m} \xi^r(x), x \in \omega^n, n \neq m. \end{array} \right. & \quad (3) \end{aligned}$$

The subspaces

$$\begin{aligned} \bigvee_{\pi^2 l^2 \delta^{-2} + V_\delta - \Lambda^F < 0} e_l & := E_+ \subset L_2(\Gamma), \\ \bigvee_{\pi^2 l^2 \delta^{-2} + V_\delta - \Lambda^F > 0} e_l & := E_- \subset L_2(\Gamma) \end{aligned}$$

are called the entrance subspaces of open and closed channels, respectively, $E_+ \oplus E_- = L_2(\Gamma)$. The subspaces $\mathcal{H}_\pm := E_\pm \times L_2(0, \infty) \in L_2(\omega)$ are called *the channel spaces* of the open and closed channels. They may be interpreted as invariant subspaces of the unperturbed Schrödinger operator l^ω in $L_2(\omega)$, defined by the restriction of the differential expression \mathcal{L} onto $L_2(\omega^{out})$ with zero boundary condition (“solid wall”) on Γ and zero boundary conditions on both shores of the leads.

Matching on Γ the scattering Ansatz $\vec{\psi}$ to the solution of the Schrödinger equation inside the quantum well gives an infinite linear system for the coefficients $S_{l,r}^n, s_{l,r}^n$, see [12]. Formally this system can be solved, if the Green function G_{int} of the Schrödinger operator L_{int} on Ω_{int} , with zero boundary condition, and Meixner conditions at the inner angles of the boundary, is constructed.

Really, according to general theory of the second order linear partial equations, see [13], the solution u of the boundary problem with the data $u \Big|_\Gamma = u_\Gamma$

is represented by the Poisson map with the Poisson kernel:

$$u(x) = \int_{\Gamma} \mathcal{P}_{int}(x, \gamma) u_{\Gamma}(\gamma) d\gamma = - \int_{\Gamma} \frac{\partial G_{int}(x, \gamma)}{\partial n_{\gamma}} u_{\Gamma}(\gamma) d\gamma \Big|_{\Gamma}.$$

The corresponding boundary current is calculated formally as

$$\frac{\partial u}{\partial n} \Big|_{\Gamma} = - \int_{\Gamma} \frac{\partial^2 G_{int}(x, \gamma)}{\partial n_x \partial n_{\gamma}} u_{\Gamma}(\gamma) d\gamma \Big|_{\Gamma} := \mathcal{DN}_{int} u_{\Gamma}.$$

The operator \mathcal{DN}_{int} is called Dirichlet-to-Neumann map of L_{int} . It is correctly defined on the appropriate Sobolev class on Γ , see [14, 15]. More about modern DN- techniques and its applications in spectral analysis can be found in [16, 17, 18, 19, 20]. In this paper we study connection between the one-body scattering matrix and the DN-map on the two-dimensional junction. For “thin” junctions the connection is used in transport problems in [11, 21, 22].

Denoting by K_{\pm} the exponents of the above Ansatz in the open and closed channels in the wires and by S, s the coefficients in front of the corresponding exponentials, we represent the Ansatz for the scattered wave on the leads in form

$$\Psi(x, \nu) = e^{iK_+x} \nu + e^{-iK_+x} S\nu + e^{-K-x} s\nu \quad (4)$$

In fact only the oscillating component of the scattered wave in the open channels contains an essential information on details of the scattering process. The direct problem of scattering is: to find the coefficients S in front of the oscillating exponentials $e^{-iK_+x} S\nu$ - the scattering matrix. In case when the solid wall is erected on the bottom sections $\Gamma = \cup_m \gamma^m$ of the wires, the Scattering matrix is $-I$. The removal of the wall results in breeding of the standing waves on the quantum well with the running exponential waves in the wires. This breeding generates the exponentially decreasing “evanescent waves” $e^{-K-x} s\nu$, which do not contribute to results of scattering at infinity, but affect the shape of the oscillating modes and add serious computational obstacles, see for instance [12].

The difficulty of the direct scattering problem is defined by the fact, that the above matching is a major perturbation of

$$L_{\Omega_{int}} \oplus l^{\omega} := \mathcal{L}_0 \longrightarrow \mathcal{L},$$

caused by the removal of the “solid wall” on Γ via replacement of the zero boundary condition by the matching condition. It is a typical perturbation

problem on continuous spectrum, for an operator \mathcal{L}_0 which has embedded eigenvalues. Breeding of the standing waves in the quantum well with the running waves in the wires gives non-square -integrable resonance states, which define resonance character of the transmission across the quantum well. Unfortunately this breeding can't be interpreted in terms of the spectral theory of self-adjoint operators. Nevertheless we are able to suggest an algebraic version of the analysis of this breeding, based on the corresponding Krein formula.

3 Krein formula for the scattering matrix

Krein formula for the scattering matrix which corresponds to the generalized resolvent of a general symmetric operator was obtained first in [27]. In [28] this formula was used in analysis of zero-range solvable models. In [3] the Krein formula is used for analysis of the one-dimensional model of the quantum network in form of a quantum graph. In this paper we aim on the problem of fitting of the model suggested in [3].

We begin with derivation of the Krein formula for the scattering matrix of a realistic two-dimensional junction. The parameters of the fitted solvable model of the junction can be selected based on comparison of the special rescription of the Krein formula of the junction, see next section, Theorem 3.1, with the corresponding formula of the model.

Consider the decomposition of the cross-section subspace $E := L_2(\Gamma)$ into an orthogonal sum of the entrance subspaces E_{\pm} of the open and closed channels. Assuming that the Dirichlet-to-Neumann map \mathcal{DN}_{int} of the Schrödinger operator L_{int} is known, construct the matrix representation of \mathcal{DN}_{int} with respect to the orthogonal decomposition $E = E_+ \oplus E_-$, denoting by P_{\pm} the corresponding orthogonal projections $I = P_+ \oplus P_-$:

$$\mathcal{DN}_{int} = \begin{pmatrix} P_+ \mathcal{DN} P_+ & P_+ \mathcal{DN} P_- \\ P_- \mathcal{DN} P_+ & P_- \mathcal{DN} P_- \end{pmatrix} := \begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix}. \quad (5)$$

The Cauchy data of the scattering Ansatz on the bottom sections Γ are:

$$\begin{aligned} \Psi(\nu) \Big|_{\Gamma} &= (I + S)\nu + s\nu, \\ \Psi'(\nu) \Big|_{\Gamma} &= iK_+(I - S)\nu - K_-s\nu, \end{aligned} \quad (6)$$

Inserting the boundary values of the Scattering Ansatz on the bottom sections into the DN-map, we obtain:

$$\begin{aligned}\mathcal{DN}\{[I+S]\nu+s\nu\} &= \\ &= iK_+[I-S]\nu - K_-s\nu.\end{aligned}$$

The orthogonal components of the result in E_{\pm} are equal to

$$\begin{aligned}\mathcal{DN}_{++}[I+S]\nu + \mathcal{DN}_{+-}s\nu &= iK_+(I-S)\nu, \\ \mathcal{DN}_{-+}[I+S]\nu + \mathcal{DN}_{--}s\nu &= -K_-s\nu,\end{aligned}$$

respectively. If $\mathcal{DN}_{--} + K_-$ is invertible on a complex neighborhood of the essential spectral interval, that gives

$$s\nu = -\frac{I}{\mathcal{DN}_{--} + K_-}\mathcal{DN}_{-+}[I+S]\nu,$$

which implies the following Krein formula for the scattering matrix, with the denominator preceding the numerator:

$$S = \frac{iK_+ - \left[\mathcal{DN}_{++} - \mathcal{DN}_{+-} \frac{I}{\mathcal{DN}_{--} + K_-} \mathcal{DN}_{-+} \right]}{iK_+ + \left[\mathcal{DN}_{++} - \mathcal{DN}_{+-} \frac{I}{\mathcal{DN}_{--} + K_-} \mathcal{DN}_{-+} \right]} \quad (7)$$

The expression

$$\mathcal{DN}_{++} - \mathcal{DN}_{+-} \frac{I}{\mathcal{DN}_{--} + K_-} \mathcal{DN}_{-+} := \mathcal{DN}^F \quad (8)$$

has a structure typical for the classical Krein formula and can be interpreted as a Dirichlet-to-Neumann map of an *intermediate Hamiltonian*, so that

$$S = \frac{iK_+ - \mathcal{DN}^F}{iK_+ + \mathcal{DN}^F}. \quad (9)$$

The formula (9) has a typical form of the scattering matrix for the one-dimensional scattering systems, see for instance [23]. Similar formula plays an important role in modern approach to the one-dimensional inverse spectral problem, see [24, 25].

To transform the Krein formula (7) of the two-dimensional scattering system to the convenient quasi-one-dimensional form (9), we have to analyze the expression (8) in details.

The intermediate Hamiltonian was introduced in [11, 21, 22] as a component L_F of the splitting

$$\mathcal{L} \longrightarrow l^F \oplus L_F$$

of \mathcal{L} defined by an additional “partial” zero boundary condition imposed at the bottom sections $\cup_m \gamma^m := \Gamma$ onto the elements from the domain of \mathcal{L} :

$$P_+ u \Big|_{\Gamma} = 0. \quad (10)$$

Here l^F , L_F are selfadjoint operators in \mathcal{H}_+ , $\mathcal{H}_- \oplus L_2(\Omega_{int})$ respectively, see [22]. The absolutely continuous spectra of l^F , L_F coincide with the union of all open and closed branches $\sigma_l = \left[\frac{\pi^2 l^2}{\delta^2} + V_{\infty}, \infty \right)$ respectively :

$$\sigma(l^F) = \cup_{open} \sigma_l, \quad \sigma_{ac}(L_F) = \cup_{closed} \sigma_l.$$

It is proven in [22], that the restriction

$$P_{L_2(\Omega_{int})} [L_F - \lambda I]^{-1} P_{L_2(\Omega_{int}) \oplus \mathcal{H}_-}$$

of the resolvent of L_F , acting as an operator from $L_2(\Omega_{int}) \oplus \mathcal{H}_-$ onto $L_2(\Omega_{int})$ can be represented by an integral operator with a kernel G^F . Then the statement (7) can be verified based on the Poisson formula for the solution of an *intermediate boundary problem* for the Schrödinger equation

$$\mathcal{L}u - \lambda u = 0, \quad P_+ u(x) = 0 \text{ if } x > 0, \quad P_+ u \Big|_{\Gamma} = u_+ \in E_+.$$

$$u(x) = - \int_{\Gamma} \frac{\partial G^F}{\partial n_{\gamma}}(x, \gamma) u_+ d\Gamma, \quad x \in \Omega_{int}.$$

Then, denoting by u_{\pm} the components of $u \Big|_{\Gamma}$ in E_{\pm} , and taking into account that $P_- \frac{\partial u}{\partial n_{\gamma}} = -K_- u_-$, we obtain:

$$\begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix} \begin{pmatrix} u_+ \\ u_- \end{pmatrix} = \begin{pmatrix} P_+ \frac{\partial u_+}{\partial n_{\gamma}} \\ -K_- u_- \end{pmatrix}.$$

One can see that the expression (8) is the Shur complement, ([26]), of the matrix

$$\begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} + K_- \end{pmatrix}$$

This implies the announced statement, once we define the DN- map of the intermediate Hamiltonian as

$$P_+ \frac{\partial u_+}{\partial n_\gamma} \Big|_\Gamma := \mathcal{DN}^F u_+. \quad (11)$$

The DN- map of the selfadjoint operator L_F has a negative imaginary part in the upper half-plane $\Im\lambda > 0$ and simple poles at the eigenvalues of L_F . Practically, for relatively thin wires, see [22], we are able to substitute the DN- map \mathcal{DN}^F in the above Krein formula (9) for the scattering matrix by the rational part

$$\mathcal{DN}^F \longrightarrow \mathcal{DN}_\Delta^F \quad (12)$$

on the essential spectral interval Δ , *with the same poles and residues on Δ* . The corresponding approximate scattering matrix takes the form

$$S(\lambda) \rightarrow S_\Delta(\lambda) = \frac{iK_+ - \mathcal{DN}_\Delta^F}{iK_+ + \mathcal{DN}_\Delta^F}. \quad (13)$$

Rational expressions of the above form (13) are typical for one-dimensional scattering systems. Sometimes they can be interpreted as scattering matrices of zero-range solvable models with “Inner Hamiltonian”, see [27, 28]. These zero-range models are automatically fitted on the essential spectral interval Δ , if \mathcal{DN}_Δ^F serves a rational approximation of \mathcal{DN}^F on Δ .

To construct the corresponding model for *arbitrary junction*, we need explicit expression for the poles and residues of the DN-map \mathcal{DN}^F of the intermediate Hamiltonian. While the corresponding data for L_{int} can be obtained via straightforward computing with standard programs, the similar problem for the intermediate Hamiltonian appears to be more difficult. Fortunately, for “relatively thin” junctions, the spectral data can be obtained via special analytic perturbation procedure based on a certain “modified” rescription of the Krein formula (8).

4 Analytic perturbation procedure for the Krein denominator and compensation of singularities.

Both terms in the left side of (8) have singularities on the spectrum of the non-perturbed operator L_{int} . It is normally expected, that the singularities of the first and second term at the eigenvalues of L_{int} compensate each other, so that only the zeros of the denominator $\mathcal{DN}_{--} + K_-$ arise as singularities of \mathcal{DN}^F . In this section we produce analysis supporting this statement, see a one-dimensional version of the statement in [31]. But we obtain in course of the relevant calculation even more important “byproduct”: we derive an algebraic equation for the eigenvalues of the intermediate Hamiltonian and calculate the residues at the corresponding poles of the intermediate DN-map. Then we are able to do the first step announced above, calculating, based on (9), the scattering matrix of a “relatively thin” junction.

For given temperature T we consider an *essential spectral interval* $\Delta_T := \Delta$, see (2). We assume that the temperature is *low*, so that Δ is situated inside the conductivity band Δ_F between the lower threshold λ_{min} of the closed channels and the upper threshold λ_{max} of the open channels

$$\Delta \subset (\lambda_{max}, \lambda_{min}) = \Delta_F.$$

Our aim is: to construct on Δ a convenient local “quasi-one-dimensional” representation of the intermediate DN-map and for the scattering matrix of the junction, (9), *with compensated singularities* inherited from the L_{int} . Later, in next section, we will use this construction as a basement for an analytic perturbation procedure, with an “intrinsic” large parameter, to calculate approximately the scattering matrix of *arbitrary* junction.

Let us present the DN-map \mathcal{DN} of L_{int} on the essential spectral interval as a sum

$$\mathcal{DN}_{int} = \sum_{\lambda_s \in \Delta} \frac{\left. \frac{\partial \varphi_s}{\partial n} \right|_{\Gamma} \left\langle \left. \frac{\partial \varphi_s}{\partial n} \right|_{\Gamma} \right\rangle}{\lambda - \lambda_s} + \mathcal{K} := \mathcal{DN}^{\Delta} + \mathcal{K} \quad (14)$$

of the rational expression constituted by the polar terms with singularities at the eigenvalues $\lambda_s \in \Delta$ of the operator L_{int} and an analytic operator-function \mathcal{K} on G_{Δ} . We will also use the operators obtained from \mathcal{DN}_{int} via framing of it by the projections P_{\pm} , for instance:

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

We introduce also the linear hull $E_\Delta = \bigvee_s \{\varphi_s\}$ - an invariant subspace of L_{int} corresponding to the essential spectral interval Δ and the part $L^\Delta := \sum_{\lambda_s \in \Delta} \lambda_s \varphi_s \langle \varphi_s$ of L_{int} in it.

To calculate the intermediate DN-map (8) in terms of the standard DN - map of L_{int} we have to solve the equation:

$$[\mathcal{DN}_{--} + K_-]u = \mathcal{DN}_{-+}g \quad (15)$$

on the essential spectral interval Δ . *It can be solved based on Banach principle if K_- can play a role of a large parameter, so that the operator*

$$[\mathcal{K}_{--} + K_-]^{-1} \quad (16)$$

exists on Δ . Then, due to continuity of \mathcal{K}_{--}, K_- there exist also a complex neighborhood of Δ where the inverse exists. We assume that this complex neighborhood is G_Δ . The junction, for which the condition (16) is fulfilled, we call *relatively thin junction*, based on the following motivation. The DN-map of L_{int} is homogeneous degree -1 . It acts from $W_2^{3/2}(\Gamma)$ to $W_2^{1/2}(\Gamma)$, see [14]. If Ω_{int} has a small diameter d then, the norm of the correcting term \mathcal{K} is estimated as $\text{Const } 1/d$. The same estimate remains true for $P_- \mathcal{K} P_- := \mathcal{K}_{--}$. The exponent K_- also acts from $W_2^{3/2}(\Gamma)$ to $W_2^{1/2}(\Gamma)$ and the norm of its inverse is estimated as $\text{Const } \delta$. Then the $W_2^{3/2}$ - norm of $K_-^{-1} \mathcal{K}_{--}$ is estimated as $\text{Const } \delta/d$. Hence, in particular, $K_- + \mathcal{K}_{--} = K_- [I + K_-^{-1} \mathcal{K}_{--}]$ is invertible if $\delta/d \ll 1$, see more comments in [22]. Notice, that for an *arbitrary junction* the auxiliary Fermi level $\Lambda_1^F := \Lambda_1$ can be selected such that the condition (16) is fulfilled. We will use this option in the following section, when calculating the scattering matrix. Now we proceed in this section assuming that (16) is fulfilled.

Denoting by T the map

$$T = \sum_{\lambda_s \in \Delta_T} \varphi_s \langle \frac{\partial \varphi_s}{\partial n},$$

and

$$T \frac{I}{\mathcal{K}_{--} + K_-} T^+ := Q(\lambda) : E_\Delta \rightarrow E_\Delta.$$

We also denote

$$\left(P_+ - \mathcal{K}_{+-} \frac{I}{\mathcal{K}_{--} + K_-} P_- \right) := \mathcal{J}(\lambda).$$

Then we discover, after some cumbersome calculation, that all singularities in the Krein formula, arising from the eigenvalues λ_s of L_{int} are compensated.

Theorem 4.1 *The Krein formula (8) for the intermediate DN - map, can be re-written, for a thin junction, on the essential spectral interval, as:*

$$\mathcal{DN}^F = \mathcal{K}_{++} - \mathcal{K}_{+-} \frac{I}{\mathcal{K}_{--} + \mathcal{K}_-} \mathcal{K}_{-+} + \mathcal{J}T^+ \rangle \frac{I}{\lambda I - L^\Delta + Q(\lambda)} \langle T\mathcal{J}^+. \quad (17)$$

The representation (17) remains valid on a complex neighborhood G_Δ of the essential spectral interval.

Remark The announced rescription (17) of the Krein formula (8) 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 of the denominator $\lambda I^\Delta - L^\Delta + Q(\lambda) := \mathcal{D}(\lambda)$:

$$\mathcal{D}(\lambda_s^F) \nu_s^F = 0.$$

These singularities coincide with the eigenvalues of the intermediate Hamiltonian. We call the above formula (17) for \mathcal{DN}^F the *modified Krein formula*. Inserting (17) into the above formula (9) gives a convenient representation for the scattering matrix of the relatively thin junction, which permits, in particular, to calculate the resonances based on eigenvalues of the intermediate operator.

In case of one-dimensional zeros of the denominator \mathcal{D} the corresponding residues are calculated as projections onto the subspaces

$$\mathcal{E}_s^F = \mathcal{J}(\lambda_s^F)T^+ \nu_s^F.$$

For multidimensional zeros of the denominator, $\mathcal{D}(\lambda_s^F)N_s^F = 0$, $\dim N_s^F > 1$ the residues are projections onto the images of the corresponding null-spaces $N_s^F = \bigvee_s \nu_s^N$

$$\mathcal{E}_s^F = \mathcal{J}(\lambda_s^F)T^+ N_s^F.$$

Proof We begin with the standard Krein formula (8) for the DN-map of the intermediate Hamiltonian L_F on the essential spectral interval Δ . Denote by \mathcal{DN}^Δ the component of the DN-map of L_{int} on Δ defined by the formula (14), and introduce similar notations for the matrix elements of \mathcal{DN} with respect to the orthogonal decomposition $E = E_+ \oplus E_-$, for instance

$$\mathcal{DN}_{+-} = \mathcal{DN}_{+-}^\Delta + \mathcal{K}_{+-}.$$

To calculate explicitly the second addendum in (8), we re-write (15) as:

$$[\mathcal{DN}_{--}^\Delta u + (K_- + \mathcal{K}_{--})] u = [\mathcal{DN}_{-+}^\Delta + \mathcal{K}_{-+}] g.$$

If $(K_- + \mathcal{K}_{--})$ is invertible on Δ , then the above equation is equivalent to:

$$\frac{I}{K_- + \mathcal{K}_{--}} \mathcal{DN}_{--}^\Delta u + u = \frac{I}{K_- + \mathcal{K}_{--}} [\mathcal{DN}_{-+}^\Delta g + \mathcal{K}_{-+}g]. \quad (18)$$

Denote

$$\frac{\langle \frac{\partial \varphi_s}{\partial n}, u \rangle}{\lambda - \lambda_s} := v_s, \quad \sum_s \varphi_s \rangle v_s = \frac{I}{\lambda I^\Delta - L^\Delta} T u := \mathbf{v},$$

and take into account that

$$\mathcal{DN}_{-+}^\Delta = P_- T^+ \frac{I}{\lambda I^\Delta - L^\Delta} T P_+.$$

Then multiplying (18) by T we obtain an equation for \mathbf{v} :

$$[\lambda I^\Delta - L^\Delta + Q(\lambda)] \mathbf{v} = Q \frac{I}{\lambda I^\Delta - L^\Delta} T P_+ g + T \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+} g.$$

This gives the following representation for \mathbf{v}

$$\mathbf{v} = \frac{I}{\lambda I^\Delta - L^\Delta + Q(\lambda)} \left[Q \frac{I}{\lambda I^\Delta - L^\Delta} T P_+ g + T \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+} g \right].$$

and permits to calculate, based on (18)

$$\begin{aligned} u = & \\ & - \frac{I}{K_- + \mathcal{K}_{--}} T^+ \mathbf{v} + \frac{I}{K_- + \mathcal{K}_{--}} T^+ \frac{I}{\lambda I^\Delta - L^\Delta} T P_+ g + \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+} g = \\ & - \frac{I}{K_- + \mathcal{K}_{--}} T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q(\lambda)} \left[Q \frac{I}{\lambda I^\Delta - L^\Delta} T P_+ g + T \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+} g \right] + \\ & \frac{I}{K_- + \mathcal{K}_{--}} T^+ \frac{I}{\lambda I^\Delta - L^\Delta} T P_+ g + \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+} g \end{aligned}$$

Now we substitute this expression into the formula (8):

$$\mathcal{DN}^F g = \mathcal{DN}_{++}^{\Delta_T} g + \mathcal{K}_{++} g - \mathcal{DN}_{+-}^{\Delta_T} u - \mathcal{K}_{+-} u = \quad (19)$$

$$P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}TP_{+g}+\mathcal{K}_{++g}-P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}TP_{-u}-\mathcal{K}_{+-u} := I_1+I_2+I_3+I_4,$$

where

$$\begin{aligned} I_3 &= -P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}TP_{-u} = \\ & -P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}Q(\lambda)\frac{I}{\lambda I^\Delta - L^\Delta}TP_{+g}- \\ & -P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}T\frac{I}{K_- + \mathcal{K}_{--}}\mathcal{K}_{-+g}+ \\ & +P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}Q\frac{I}{\lambda I^\Delta - L^\Delta + Q}Q\frac{I}{\lambda I^\Delta - L^\Delta}TP_{+g}+ \\ P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}Q\frac{I}{\lambda I^\Delta - L^\Delta + Q}T\frac{I}{K_- + \mathcal{K}_{--}}\mathcal{K}_{-+g} &= I_{31} + I_{32} + I_{33} + I_{34}, \end{aligned}$$

and

$$\begin{aligned} I_4 &= -\mathcal{K}_{+-u} = \\ & \mathcal{K}_{+-}\frac{I}{K_- + \mathcal{K}_{--}}T^+\frac{I}{\lambda I^\Delta - L^\Delta + Q(\lambda)}Q\frac{I}{\lambda I^\Delta - L^\Delta}TP_{+g}+ \\ & \mathcal{K}_{+-}\frac{I}{K_- + \mathcal{K}_{--}}T^+\frac{I}{\lambda I^\Delta - L^\Delta + Q(\lambda)}T\frac{I}{K_- + \mathcal{K}_{--}}\mathcal{K}_{-+g}+ \\ & -\mathcal{K}_{+-}\frac{I}{K_- + \mathcal{K}_{--}}T^+\frac{I}{\lambda I^\Delta - L^\Delta}TP_{+g} - \mathcal{K}_{+-}\frac{I}{K_- + \mathcal{K}_{--}}\mathcal{K}_{-+g} = \\ & I_{41} + I_{42} + I_{43} + I_{44}. \end{aligned}$$

Insert these results into the above formula (19) and collect the terms in the right side which contain the second power of $[\lambda I^\Delta - L^\Delta]^{-1}$:

$$\begin{aligned} I_{31} + I_{33} &= -P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}Q(\lambda)\frac{I}{\lambda I^\Delta - L^\Delta}TP_{+g}+ \\ & +P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}Q\frac{I}{\lambda I^\Delta - L^\Delta + Q}Q\frac{I}{\lambda I^\Delta - L^\Delta}TP_{+g} = \\ & -P_+T^+\frac{I}{\lambda I^\Delta - L^\Delta}\frac{I}{\lambda I^\Delta - L^\Delta + Q}TP_{+g}. \end{aligned} \tag{20}$$

This result, combined with I_1 yields:

$$\begin{aligned}
P_+T^+ \frac{I}{\lambda I^\Delta - L^\Delta} TP^+g - P_+T^+ \frac{I}{\lambda I^\Delta - L^\Delta} \frac{I}{\lambda I^\Delta - L^\Delta + Q} TP_+g = \\
P_+T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q} TP_+g := J_1g. \tag{21}
\end{aligned}$$

Now we combine the terms $I_{32} + I_{34}$ and $I_{41} + I_{43}$ containing $[\lambda I^\Delta - L^\Delta]^{-1}$:

$$\begin{aligned}
I_{32} + I_{34} = -P_+T^+ \frac{I}{\lambda I^\Delta - L^\Delta} \left[-I + Q \frac{I}{\lambda I^\Delta - L^\Delta + Q} \right] T \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+}g = \\
-P_+T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q} T \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+}g := J_2g, \tag{22}
\end{aligned}$$

$$\begin{aligned}
I_{41} + I_{43} = \mathcal{K}_{+-} \frac{I}{K_- + \mathcal{K}_{--}} T^+ \left[-I + \frac{I}{\lambda I^\Delta - L^\Delta + Q} Q \right] TP_+g = \\
-\mathcal{K}_{+-} \frac{I}{K_- + \mathcal{K}_{--}} T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q} TP_+g := J_3g. \tag{23}
\end{aligned}$$

We see that no terms left in the right side of (19) with singularities $[\lambda I^\Delta - L^\Delta]^{-1}$ inherited from the unperturbed operator - all these singularities are compensated. Assembling separately the terms J_1g, J_2g, J_3g, I_{43} containing $[\lambda I^\Delta - L^\Delta + Q]^{-1}$ and regular terms I_2, I_{44} , we obtain the announced expression $\mathcal{DN}^F g$

$$\begin{aligned}
\mathcal{DN}^F g = P_+T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q} TP_+g - \\
P_+T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q} T \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+}g - \\
\mathcal{K}_{+-} \frac{I}{K_- + \mathcal{K}_{--}} T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q} TP_+g + \\
\mathcal{K}_{+-} \frac{I}{K_- + \mathcal{K}_{--}} T^+ \frac{I}{\lambda I^\Delta - L^\Delta + Q(\lambda)} T \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+}g + \\
\mathcal{K}_{++}g - \mathcal{K}_{+-} \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+}g = \\
P_+T^+ - \mathcal{K}_{+-} \frac{I}{K_- + \mathcal{K}_{--}} T^+ \left. \frac{I}{\lambda I^\Delta - L^\Delta + Q(\lambda)} \right\langle TP_+ - T \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+}g +
\end{aligned}$$

$$\mathcal{K}_{++}g - \mathcal{K}_{+-} \frac{I}{K_- + \mathcal{K}_{--}} \mathcal{K}_{-+}g \quad (24)$$

The announced expression (17) for \mathcal{DN}^F is obtained from the above formula by introducing the notation $P_+ - \mathcal{K}_{+-} \frac{I}{K_- + \mathcal{K}_{--}} := \mathcal{J}$. The derived formula is extended onto the complex neighborhood G_Δ of the essential spectral interval due to analyticity. Further analytical continuation is possible as well, but the estimates of leading and subordinate terms are obviously lost.

The end of the proof

The scattering matrix of the original problem on the essential spectral interval may be obtained via replacement in (9) the intermediate DN-map by the expression (17) 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 \mathcal{K}_{--} of the rational approximation \mathcal{DN}^Δ of \mathcal{DN} . This condition may be not satisfied for given Fermi level $\Lambda := \Lambda_0$.

5 Intrinsic large parameter and an analytic perturbation procedure for the scattering matrix of an arbitrary junction

In fact the choice of the “technical” Fermi level $\Lambda^F := \Lambda_0$ is in our hands, so we are able to select another value $\Lambda_1 \gg \Lambda_0$, such that the condition (16) is fulfilled. The corresponding splitting of the original Hamiltonian would be defined by the orthogonal decomposition of the entrance space $E = [E_+^0 \oplus E_+^1] \oplus E_-$, such that few closed channels with thresholds $V_\infty + \frac{\pi^2 l^2}{\delta^2}$ situated between Λ_0 and Λ_1 are formally included into the lower group of channels, with an extended entrance subspace $E_+^0 \oplus E_+^1 := E_+$. We will use hereafter the intermediate DN-map \mathcal{DN}^1 of the operator L_1 , defined by the semi-transparent boundary condition *hight* Λ_1 associated with the above decomposition of the entrance space $L_2(\Gamma) = [E_+^0 \oplus E_+^1] \oplus E_-$.

$$P_+ u \Big|_\Gamma = 0, \text{ with } P_+ := P_{E_+^0 \oplus E_+^1}.$$

Denote by K_+^0, K_\pm^1 the exponents of the oscillating and decreasing solutions of the Schrödinger equation in the channels associated with E_+^0, E_\pm^1 , respectively.

Consider the orthogonal decomposition $E = E_+^0 \oplus E_+^1 \oplus E_-^1$ and represent the DN-map \mathcal{DN} of L_{int} by the matrix

$$\mathcal{DN} = \begin{pmatrix} \mathcal{DN}_{++}^{00} & \mathcal{DN}_{++}^{01} & \mathcal{DN}_{+-}^{01} \\ \mathcal{DN}_{++}^{10} & \mathcal{DN}_{++}^{11} & \mathcal{DN}_{+-}^{11} \\ \mathcal{DN}_{-+}^{10} & \mathcal{DN}_{-+}^{11} & \mathcal{DN}_{--}^{11} \end{pmatrix} := \mathbf{DN}. \quad (25)$$

Hereafter we consider the Schrödinger operator (1) on an *arbitrary* junction $\Omega = \Omega_{int} \cup \omega$, assuming that the compact domain Ω_{int} has a piecewise smooth boundary and the Meixner conditions are imposed at the inner corners of the boundary of Ω_{int} . Consider the rational approximation of the DN-map of the Schrödinger operator L_{int} on the essential spectral interval Δ :

$$\mathcal{DN} = \mathcal{DN}(\Delta) + \mathcal{K},$$

including into $\mathcal{DN}(\Delta)$ the polar terms corresponding to the eigenvalues $\lambda_s \in \Delta$:

$$\sum_{\lambda_s \in \Delta} \frac{\langle \frac{\partial \varphi_s}{\partial n} \rangle \langle \frac{\partial \varphi_s}{\partial n} \rangle}{\lambda - \lambda_s} =: \mathcal{DN}(\Delta),$$

with a properly selected self-adjoint operator C_Δ and denote appropriately the corresponding matrix elements, for instance:

$$\mathcal{DN}_{++}^{00} = \mathcal{DN}(\Delta)_{++}^{00} + \mathcal{K}_{++}^{00}.$$

Now we select, for the junction Ω , the technical Fermi-level Λ_1 from the condition, that the junction is thin, with respect to the new Fermi level Λ_1 :

Definition *We say that the quantum network is relatively thin on the level Λ_1 if the operator $\mathcal{K}_{--}^{11} + K_-^1$ is invertible on some complex neighborhood G_Δ of the essential spectral interval Δ .*

This condition may be substituted by a stronger, but more convenient condition

$$\sup_{\lambda \in G_\Delta} \|\mathcal{K}_{+-}^{00}(\lambda)\| < \sqrt{\Lambda_1^F - \Lambda^F - 2m_0 \kappa T \hbar^{-2}}. \quad (26)$$

If Λ_1 is defined from (26), we construct the corresponding decomposition $E = E_+ \oplus E_-$, with $E_+ = [E_+ \oplus E_+^1]$, $E_- = E_-^1$

$$E = [E_+^0 \oplus E_+^1] \oplus E_-^1.$$

and define the intermediate Hamiltonian L_1 as a non-trivial component of the corresponding splitting of \mathcal{L} :

$$\mathcal{L} = L_F^1 \oplus l_1^F, \quad (27)$$

obtained by imposing on Γ the additional boundary condition

$$P_+ u \Big|_{\Gamma} = 0.$$

Note that the trivial part l_1^F of this splitting contains additional channels in the “lover” group of channels : $E_+ = E_+^0 \oplus E_+^1$, which correspond to exponentially decreasing modes $e^{-K_+^1 x} \nu$. The matrix (25) connects the boundary data $\Psi(0)$, $\Psi'(0)$ of the scattering Ansatz

$$\Psi(x, \lambda) = e^{iK_+ x} \nu + e^{-iK_+ x} S \nu + e^{-K_+^1 x} s_+^1 \nu + e^{-K_-^1 x} s_-^1 \nu, \quad (28)$$

$$\begin{pmatrix} iK_+(\nu - S\nu) \\ -K_+^1 s_+^1 \nu \\ -K_-^1 s_-^1 \nu \end{pmatrix} = \mathbf{DN} \begin{pmatrix} (\nu + S\nu) \\ s_+^1 \nu \\ s_-^1 \nu \end{pmatrix}$$

Eliminating $s_-^1 \nu$ from the last equation,

$$s_-^1 \nu = \frac{I}{\mathcal{DN}_{--}^{11} + K_-^1} [\mathcal{DN}_{-+}^{01}(\nu + S\nu) + \mathcal{DN}_{-+}^{11} s_+^1 \nu]$$

we obtain a *finite-dimensional equation for the components of the scattering Ansatz in $E_+^0 \oplus E_+^1$*

$$\begin{pmatrix} iK_+(\nu - S\nu) \\ -K_+^1 s_+^1 \nu \end{pmatrix} = \tilde{\mathbf{DN}} \begin{pmatrix} (\nu + S\nu) \\ s_+^1 \nu \end{pmatrix}.$$

Here

$$\tilde{\mathbf{DN}} := \begin{pmatrix} \tilde{\mathcal{DN}}_{++}^{00} & \tilde{\mathcal{DN}}_{++}^{01} \\ \tilde{\mathcal{DN}}_{++}^{10} & \tilde{\mathcal{DN}}_{++}^{11} \end{pmatrix},$$

where

$$\begin{aligned} \tilde{\mathcal{DN}}_{++}^{00} &= \mathcal{DN}_{++}^{00} - \mathcal{DN}_{+-}^{01} \frac{I}{\mathcal{DN}_{--}^{11} + K_-^1} \mathcal{DN}_{-+}^{10}, \\ \tilde{\mathcal{DN}}_{++}^{01} &= \mathcal{DN}_{++}^{01} - \mathcal{DN}_{+-}^{01} \frac{I}{\mathcal{DN}_{--}^{11} + K_-^1} \mathcal{DN}_{-+}^{11}, \end{aligned}$$

$$\begin{aligned}\tilde{\mathcal{D}}\mathcal{N}_{++}^{10} &= \mathcal{D}\mathcal{N}_{++}^{10} - \mathcal{D}\mathcal{N}_{+-}^{11} \frac{I}{\mathcal{D}\mathcal{N}_{--}^{11} + K_-^1} \mathcal{D}\mathcal{N}_{-+}^{10}, \\ \tilde{\mathcal{D}}\mathcal{N}_{++}^{11} &= \mathcal{D}\mathcal{N}_{++}^{11} - \mathcal{D}\mathcal{N}_{+-}^{11} \frac{I}{\mathcal{D}\mathcal{N}_{--}^{11} + K_-^1} \mathcal{D}\mathcal{N}_{-+}^{11}.\end{aligned}$$

Eliminating $s_+^1 \nu$ from the second equation we obtain a finite-dimensional expression for the Scattering matrix of the junction

$$S(\lambda) = \frac{iK_+ - \left[\tilde{\mathcal{D}}\mathcal{N}_{++}^{00} - \tilde{\mathcal{D}}\mathcal{N}_{++}^{01} \frac{I}{\tilde{\mathcal{D}}\mathcal{N}_{++}^{11} + K_+^1} \tilde{\mathcal{D}}\mathcal{N}_{++}^{01} \right]}{iK_+ + \left[\tilde{\mathcal{D}}\mathcal{N}_{++}^{00} - \tilde{\mathcal{D}}\mathcal{N}_{++}^{01} \frac{I}{\tilde{\mathcal{D}}\mathcal{N}_{++}^{11} + K_+^1} \tilde{\mathcal{D}}\mathcal{N}_{++}^{01} \right]}, \quad (29)$$

with the denominator preceding the numerator. The ultimate representation (29) of the scattering matrix is completely finite-dimensional, hence more convenient for the computational process. The large parameter Λ_1 permits to eliminate the infinite-dimensional part K_-^1 of K_- and obtain a completely finite-dimensional formula (29) for the scattering matrix, without any additional assumptions on geometrical or physical parameters of the network. Actually essential details of the analytic perturbation process which are still present in (7) are mostly reloaded by (29) on the direct computing with finite matrices. Hence the formula (29) opens, in particular, a semi-analytic way of calculating of transmission coefficients across any junction. Comparison of the formula (29) with (9) implies the equation

$$\tilde{\mathcal{D}}\mathcal{N}_{++}^{00} - \tilde{\mathcal{D}}\mathcal{N}_{++}^{01} \frac{I}{\tilde{\mathcal{D}}\mathcal{N}_{++}^{11} + K_+^1} \tilde{\mathcal{D}}\mathcal{N}_{++}^{01} = \mathcal{D}\mathcal{N}^F. \quad (30)$$

The terms of (30) contain sophisticated singularities inherited from the operator L_{int} . Again, we are able to transform this expression to another form, with all singularities compensated. We observe first the compensation singularities in \mathbf{DN} , representing it Krein's form. Denote

$$\begin{aligned}\mathcal{T}_+ &= \sum_{\lambda_s \in \Delta} \varphi_s \langle P_+^0 \frac{\partial \varphi_s}{\partial n} + P_+^1 \frac{\partial \varphi_s}{\partial n}, \\ \mathcal{T}_- &= \sum_{\lambda_s \in \Delta} \varphi_s \langle P_-^1 \frac{\partial \varphi_s}{\partial n},\end{aligned}$$

and consider the rational approximation of \mathbf{DN}

$$\mathbf{DN} = \mathbf{DN}(\Delta) + \mathcal{K} :$$

$$\mathbf{DN}_{++} := \begin{pmatrix} \mathcal{DN}_{++}^{00} & \mathcal{DN}_{++}^{01} \\ \mathcal{DN}_{++}^{10} & \mathcal{DN}_{++}^{11} \end{pmatrix} = \mathcal{T}_+^+ \frac{I}{\lambda I^\Delta - L^\Delta} \mathcal{T}_+ + \begin{pmatrix} \mathcal{K}_{++}^{00} & \mathcal{K}_{++}^{01} \\ \mathcal{K}_{++}^{10} & \mathcal{K}_{++}^{11} \end{pmatrix},$$

$$\mathbf{DN}_{+-} := \begin{pmatrix} \mathcal{DN}_{+-}^{00} & \mathcal{DN}_{+-}^{01} \\ \mathcal{DN}_{+-}^{10} & \mathcal{DN}_{+-}^{11} \end{pmatrix} = \mathcal{T}_+^+ \frac{I}{\lambda I^\Delta - L^\Delta} \mathcal{T}_- + \begin{pmatrix} \mathcal{K}_{+-}^{01} \\ \mathcal{K}_{+-}^{11} \end{pmatrix},$$

$$\mathbf{DN}_{-+} := \begin{pmatrix} \mathcal{DN}_{-+}^{10} & \mathcal{DN}_{-+}^{11} \\ \mathcal{DN}_{-+}^{01} & \mathcal{DN}_{-+}^{00} \end{pmatrix} = \mathcal{T}_-^+ \frac{I}{\lambda I^\Delta - L^\Delta} \mathcal{T}_+ + (\mathcal{K}_{-+}^{10}, \mathcal{K}_{-+}^{11}),$$

Consider the Krein formula for $\tilde{\mathbf{DN}}$

$$\tilde{\mathbf{DN}} = \mathbf{DN}_{++} - \mathbf{DN}_{+-} \frac{I}{\mathcal{DN}_{--}^{11}(\Delta) + \mathcal{K}_{--}^{11} + K_-^1} \mathbf{DN}_{-+}. \quad (31)$$

Compensation of singularities in (31) inherited from the spectrum of L_{int} can be observed in the same way as the compensation of singularities in (8). Introduce

$$\mathcal{T}_{+-} \frac{I}{\mathcal{K}_{--} + K_-} \mathcal{T}_{-+}^+ := Q(\lambda) : E_\Delta \rightarrow E_\Delta,$$

and

$$P_+ - \begin{pmatrix} \mathcal{K}_{+-}^{01} \\ \mathcal{K}_{+-}^{11} \end{pmatrix} \frac{I}{\mathcal{K}_{--}^{11} + K_-^1} P_- := \mathcal{J}(\lambda).$$

Theorem 5.1 *The Krein formula (31) for the $\tilde{\mathbf{DN}}$ can be re-written on the essential spectral interval, as:*

$$\begin{aligned} \tilde{\mathbf{DN}} &= \begin{pmatrix} \mathcal{K}_{++}^{00} & \mathcal{K}_{++}^{01} \\ \mathcal{K}_{++}^{10} & \mathcal{K}_{++}^{11} \end{pmatrix} - \begin{pmatrix} \mathcal{K}_{+-}^{01} \\ \mathcal{K}_{+-}^{11} \end{pmatrix} \frac{I}{\mathcal{K}_{--}^{11} + K_-^1} (\mathcal{K}_{-+}^{01}, \mathcal{K}_{-+}^{11}) + \\ &\quad \mathcal{J} T^+ \rangle \frac{I}{\lambda I - L^\Delta + Q(\lambda)} \langle T \mathcal{J}^+ = \mathcal{K}_\Delta^F + \mathcal{DN}_\Delta^F, \end{aligned} \quad (32)$$

with

$$\mathcal{K}_\Delta^F := \begin{pmatrix} \mathcal{K}_{++}^{00} & \mathcal{K}_{++}^{01} \\ \mathcal{K}_{++}^{10} & \mathcal{K}_{++}^{11} \end{pmatrix} - \begin{pmatrix} \mathcal{K}_{+-}^{01} \\ \mathcal{K}_{+-}^{11} \end{pmatrix} \frac{I}{\mathcal{K}_{--}^{11} + K_-^1} (\mathcal{K}_{-+}^{01}, \mathcal{K}_{-+}^{11})$$

and

$$\mathcal{DN}_\Delta^F := \mathcal{J} T^+ \rangle \frac{I}{\lambda I - L^\Delta + Q(\lambda)} \langle T \mathcal{J}^+ = \sum_{\lambda_s^F} \frac{\phi_s^F \rangle \langle \phi_s^F}{\lambda - \lambda_s^F}. \quad (33)$$

Here λ_s^F are the eigenvalues of the intermediate Hamiltonian which arose from the eigenvalues of L_{int} on the essential spectral interval, and ϕ_s^F are the projections of the boundary currents of the corresponding normalized eigenfunctions φ_s^F of the intermediate Hamiltonian L^F onto the entrance subspace E_+ of the open channels,

$$\phi_s^F = P_+ \frac{\partial \varphi_s^F}{\partial n} \Big|_{\Gamma}.$$

The summation on s in the above formula (33) is spread over all (vector-) zeros of $L^\Delta - \lambda I^\Delta + Q(\lambda)$ which arose from the eigenvalues of L_{int} on the essential spectral interval. The representation (31) remains valid on some complex neighborhood G_Δ of the essential spectral interval.

Note that the expression (30) is the Schur complement, see [26], of the matrix

$$\tilde{\mathbf{D}}\mathbf{N} + \begin{pmatrix} 0 & 0 \\ 0 & K_-^1 \end{pmatrix} = \begin{pmatrix} \mathcal{DN}_{++}^{00} & \mathcal{DN}_{++}^{01} \\ \mathcal{DN}_{++}^{10} & \mathcal{DN}_{++}^{11} + K_-^1 \end{pmatrix}.$$

Absence of singularities at the spectrum of L_{int} in (32) is inherited by the Schur complement. Inserting the Schur complement into (29) gives an explicit formula for the scattering matrix of the junction in form:

$$S(\lambda) = \{iK_+ - [\mathcal{DN}_\Delta^F + \mathcal{K}_\Delta^F]\} \{iK_+ + [\mathcal{DN}_\Delta^F + \mathcal{K}_\Delta^F]\}^{-1}, \quad (34)$$

with the denominator preceding the numerator. The details of this representation can be recovered, if needed, from the above theorem 5.1. We leave this calculation to the reader. Note that the above expression (34) for the scattering matrix can be simplified if some additional assumption is imposed on K_+ , \mathcal{K}_Δ^F .

Definition We call the junction Ω *thin in open channels on the essential spectral interval* if

$$\| K_+^{-1/2} \| \| K_+^{-1/2} \mathcal{K}_\Delta^F \| < 1.$$

Theorem 5.2 *If the junction Ω is thin in open channels on the essential spectral interval, then it can be obtained by the analytic perturbation procedure from the essential scattering matrix*

$$S_{ess}(\lambda) = [iK_+ - \mathcal{DN}_\Delta^F][iK_+ + \mathcal{DN}_\Delta^F]^{-1}, \quad (35)$$

where denominator precedes the numerator and the intermediate DN-map $\mathcal{DN}^F = \mathcal{DN}_\Delta^F + \mathcal{K}_\Delta^F$ is substituted by the essential polar part \mathcal{DN}_Δ^F .

Proof Represent the numerator and the denominator of the right side of (34) as:

$$iK_+ - [\mathcal{DN}_\Delta^F + \mathcal{K}_\Delta^F] = (iK_+ - \mathcal{DN}_\Delta^F) \left[I - (iK_+ - \mathcal{DN}_\Delta^F)^{-1} \mathcal{K}_\Delta^F \right]$$

$$iK_+ + [\mathcal{DN}_\Delta^F + \mathcal{K}_\Delta^F] = (iK_+ + \mathcal{DN}_\Delta^F) \left[I + (iK_+ + \mathcal{DN}_\Delta^F)^{-1} \mathcal{K}_\Delta^F \right].$$

Notice that

$$\sup_{\lambda \in \Delta} \| (iK_+ + \mathcal{DN}_\Delta^F)^{-1} \mathcal{K}_\Delta^F \| < 1, \quad (36)$$

if

$$\| K_+^{-1/2} \| \| K_+^{-1/2} \mathcal{K}_\Delta^F \| < 1$$

Indeed, denote $\mathcal{DN}_\Delta^F := A$, $\mathcal{K}_\Delta^F := B$. Then

$$\begin{aligned} \left\| \frac{I}{iK_+ + A} B u \right\| &\leq \left\| K_+^{-1/2} \frac{I}{iI + K_+^{-1/2} A K_+^{-1/2}} K_+^{-1/2} B u \right\| \leq \\ &\| K_+^{-1/2} \| \left\| \frac{I}{iI + K_+^{-1/2} A K_+^{-1/2}} K_+^{-1/2} B u \right\| \leq \| K_+^{-1/2} \| \| K_+^{-1/2} B u \| \leq \\ &\| K_+^{-1/2} \| \| K_+^{-1/2} \mathcal{K}_\Delta^F u \|. \end{aligned}$$

This result implies (36). Now we can represent the scattering matrix as a product of three factors:

$$\begin{aligned} S(\lambda) = & \left[I + (iK_+ + \mathcal{DN}_\Delta^F)^{-1} \mathcal{K}_\Delta^F \right]^{-1} S_{ess}(\lambda) \left[I - (iK_+ - \mathcal{DN}_\Delta^F)^{-1} \mathcal{K}_\Delta^F \right]. \quad (37) \end{aligned}$$

The central factor coincides with the essential scattering matrix, and the left and right factors contain the small parameter $(iK_+ \pm \mathcal{DN}_\Delta^F)^{-1} \mathcal{K}_\Delta^F$. Hence the first factor can be decomposed into the geometrically convergent series. Thus the scattering matrix can be obtained from the essential scattering matrix via standard analytic perturbation procedure, with the above small parameter.

The end of the proof

Remark 1 Denote by λ_0 the vector zero of the numerator of the essential scattering matrix:

$$[iK_+ - \mathcal{DN}_\Delta^F] e_0 = 0.$$

For the network which is *sufficiently thin* on the open channels the estimate

$$\sup_{\lambda \in \Sigma_\epsilon} \| [iK_+ - \mathcal{DN}_\Delta^F]^{-1} \mathcal{K}_\Delta^F \| < 1$$

is valid on a small circle $\Sigma_\epsilon = \{|\lambda - \lambda_0| = \epsilon\}$ centered at λ_0 . Then, due to the operator-valued Rouché theorem, [34] the numerators of the original and the essential scattering matrices have equal total multiplicity of vector zeros inside Σ_ϵ , because

$$\sup_{\Sigma_\epsilon} \| I - [iK_+ - \mathcal{DN}_\Delta^F]^{-1} [iK_+ - \mathcal{DN}_\Delta^F - \mathcal{K}_\Delta^F] \| =$$

$$\sup_{\Sigma_\epsilon} \| [iK_+ - \mathcal{DN}_\Delta^F]^{-1} \mathcal{K}_\Delta^F \| < 1.$$

Thus the zeros of the original scattering matrix - resonances - of the thin junction are situated close to the zeros of the essential scattering matrix. A relevant perturbation procedure may be developed for calculation of the resonances. Localization of zeros is important for estimation of speed of transition processes in the junction, if it is used as a switch.

Remark 2 The above statement (35) and the formula (37) permits to substitute, on the essential spectral interval, the scattering matrix of a thin junction by the essential scattering matrix. According to [30], the essential scattering matrix can be interpreted as a Scattering matrix of a solvable model.

6 Conclusion: role of solvable models in analytic perturbation procedure and a relevant realization problem

The solvable model of thin junction fitted on a certain essential spectral interval can serve as a first step of - *jump-start*, see [29] - of the modified analytic perturbation procedure which is applied to perturbation of embedded eigenvalues, see extended comments in [22]. The proposed jump-start procedure confirms the hypothesis of H. Poincaré, about the role of resonances in analytic perturbation procedure: elimination, due to the chain-rule for the scattering matrices, of resonances on the essential spectral interval Δ permits to

construct a convergent analytic perturbation procedure. Unfortunately neither *finite* degree of precision in our approximations for the scattering matrix allows to construct the solvable model with exactly the same resonances on Δ as in original scattering problem. Nevertheless one can say, that zero-range solvable models of the quantum system, see for instance [36, 37, 38, 39] could, after appropriate fitting, play a role of the jump start. Our jump-start solvable models, see also [29, 30, 40, 41, 22] are automatically fitted, because the corresponding scattering matrix serves an approximation of the whole scattering matrix of the original perturbed operator.

It may be interesting that Nobel Prize winner 1972 Iliya Prigogine, see [42], inspired by the above mentioned idea of H. Poincare, [35], about the role of resonances in analytic perturbation procedure, attempted to construct an “intermediate operator”- a version of our jump-start- as a tool of analytic perturbation procedure on continuous spectrum. His attempt was not successful, because he imposed, in advance, too strong conditions on the object of his search. In particular, he assumed that the intermediate operator should be a function of the non-perturbed Hamiltonian. Our jump-start is obtained based on local rational approximation of the corresponding DN-map, and it is constructed via finite-dimensional perturbation of the original Hamiltonian, with the same leading resonances on the essential spectral interval.

We were able, see sections 4,5 and references therein, to construct a solvable model of a *thin junction* in the Hilbert space with a standard positive metric. We conjecture, that a similar solvable model can be constructed for *arbitrary junction* when using operators in Pontryagin space based on the corresponding realization theorems, see for instance [43]. Note that solvable models in Pontryagin space are more flexible, but yet reduce to a standard selfadjoint operators in the positive invariant subspace of scattered waves, see for instance [40, 41].

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