NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2010, VOL. 1, No. 1, P. 108–147

**UDC 517.9**

# RESONANCE ONE-BODY SCATTERING ON A JUNCTION

G. Martin[1], A. M. Yafyasov[2], B. S. Pavlov[1,2]

[1] NZ institute for Advanced study, Massey University, Auckland, New Zealand
[2] V. Fock Institute for Physics at the St. Petersbourg University, Russia
pavlovenator@gmail.com

In this paper we propose a synthesis of various approaches mixing computational modeling, solving complex and sometimes ill-posed inverse problems and the development of efficient analytic perturbation procedures, which offer an analytic path to the solution of the mathematical design and optimization problems for constructing quantum networks with prescribed transport properties. We consider the simplest sort of $2D$ quantum networks — the junctions — and focus on the problems of the resonance scattering, caused by the spectral properties of the relevant Schrödinger operator on the vertex domain. Typically, 1-D features appear in the form of the single-mode scattering on the first spectral (energy) band in the resulting solvable model, but the analysis of multi-mode scattering is possible with our methodology. However, this comes at the price of assuming realistic (as opposed to quite general) matching between the scattering Ansatz in the wires and the solution of the Schrödinger equation on the vertex domain. Here this matching is based on a recently developed version of the Dirichlet-to-Neumann map. We are further able to observe the transformation of the discrete spectrum of the Schrödinger operator on the vertex domain into the resonance features of the relevant scattering problem.

**Keywords:** scattering, junction.

## 1. Quantum Networks: physical background, motivation and the road map

Computational investigation and computer based modeling are an unavoidable component of much of modern scientific research. Increasing demands to handle large data sets more quickly, or computationally solve extremely large systems of equations, or more and more complicated PDEs do not align well with the demand for more compact constructions, greater speed or other efficiencies. Indeed, the only way forward from where we are at the moment seems to rest on the development of fast nano-size elements of a quantum nature. Silicon based technology is unlikely to meet the needs of future generations of researchers and is already basically outdated since nano-size elements (produced by known classical technology) require large scale low-temperature equipment without offering the speed improvements.

The international community of computer engineers and materials scientists have focussed on the search for new cheap and technologically flexible materials which would replace silicon in manufacturing elements of computers of the next generation. However, it is already clear that the search for new materials must go hand in hand with the search for new design of elements, new working regimes and new technology. It is fair to say that the international research community expects that the classical designs, working regimes and technology of manufacturing soon will be replaced by the corresponding “quantum” analogs.

Quantum networks belong to a wider class of resonance scattering systems. According to [1], even in simplest case of linear transport processes, these systems are described by linear differential equations, e.g the wave equation or the Schrödinger equation, on special domains admitting a subdivision into two parts: a linear equation ( Schrödinger equation ) on the region surrounded by barriers ( e.g. a quantum well ) and a similar equation on a reservoir, the two being weakly coupled by tunneling, see for instance or by a thin channel. The typical example of the latter system is provided by the classical Helmholtz Resonator, see [2] and references

therein. In the case of Quantum Network this decomposition corresponds, see [1], is reduced to the "schematization of the transport process as a coherent process on the quantum well, fed by the exterior reservoirs" - in our case the role of reservoirs played by the quantum wires . On the reservoirs, assumed to be homogeneous and neutral, the electron - electron interaction is usually 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. Validity of a $1D$ quantum graph for approximate description of the dynamics of electrons on the $2D$ quantum network inspired a number of papers, see for instance [3–8], where actually the small energy asymptotic of spectral properties of the Laplacian on the network is studied. Another series of papers [9–14] is aimed to the spectral properties of Laplacean on the manifolds with cusps.

The quantum mechanics was already well developed through the 20-th century to understand physics of atoms and molecules, and even to verify numerically basic physical parameters, even though it still seems far from the demands of standard engineering practices. Unfortunately, the basic equations of quantum mechanics admit explicit solutions only in rare cases. Hence the optimization of the design of elements of quantum devices with prescribed properties and functions now requires: either

- significant computational modeling, including scanning over highly multidimensional spaces of all essential physical and geometrical parameters affecting the final properties of the device engineered,
- or solving extraordinary complex and sometimes ill-posed inverse problems, which would connect directly the required functions and properties of the quantum devices with the basic physical and geometrical parameters,
- or development of efficient analytic perturbation procedures, offering an analytic path to the solution of the mathematical design and optimization problems for the corresponding "quantum networks".

None of these design optimisation processes developed separately could provide a complete and viable solution to all the engineering problems for every quantum network. In this paper, we propose a synthesis of the these approaches to construct a procedure of mathematical design of a quantum network with prescribed transport properties.

We consider the simplest sort of 2-D quantum networks - the junctions- constructed of the 2-D vertex domains (quantum wells, quantum dots), $\Omega_s$, and straight 2-D leads (quantum wires), $\omega^m$, all of equal width $\delta$ connecting the wells to each other or possibly extending to infinity. In contrast with earlier attempts as noted above, we pay close attention to the dynamics and geometry on the vertex domains and the potential of the corresponding Schrödinger equation.

It is convenient to assume that the domains and the leads are separated from each other by imaginable bottom sections $\gamma_m$ orthogonal to the axes of the quantum wires - as illustrated - with $\bigcup_m \ \gamma_m = \Gamma$,

A reasonably strong quantum current will be formed by a huge number of electrons and so the transport problem on the quantum network needs multi-particle quantum mechanics. Unfortunately, currently this multi-particle technique has been developed only for domains in $\mathbb{R}^n$ with trivial geometry, for instance the whole space, a half-space or possibly a cone.

The density of electrons in a solid (semiconductor) is about $10^{19} \ \ (cm)^{-1}$, thus the distance between them is about $10^{-6} \ cm$ which is typically at least two orders of magnitude larger than the minimal period in the solid. Nevertheless, the interaction between electrons cannot be neglected since various collective effects for the whole system of electrons in the solid are caused by the long-range Coulomb interaction. A practical understanding of the multi-particle aspect on a quantum network might follow the ideology of coupled clusters theory, see for instance [20] and references therein. Anyway, the basic building blocks of the multi-particle spectral

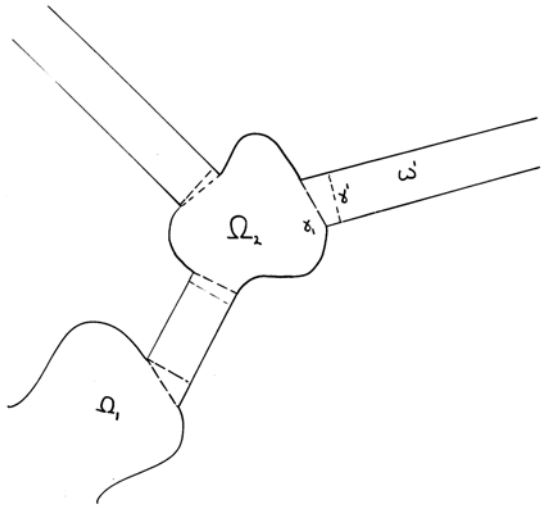


FIG. 1. A quantum 2-D network

theory are solutions of the corresponding one-body Schrödinger equations. The Slater determinant constructed from the one-body orbitals satisfy the linear multi-particle Schrödinger equation for non-interacting electrons forming multi-particle orbitals governed by the Pauli principle and possessing certain appropriate statistical properties. This linear equation can be equipped with a Coulomb interaction between electrons. The modern practice of Quantum Chemistry shows already that when a two body interaction is taken into account we obtain a realistic multi-particle spectral picture and the corresponding dynamics. This observation was confirmed, see [15], in a rigorous analysis of the zero-range model of multi-particle system with only two-body collisions taken into account.

A rigorous few body quantum mechanics on a quantum network is not developed yet, though there are few recent papers concerning two-body solvable models for 1d quantum networks. The difficulty of the problem appears from the highly inconvenient multi-particle configuration space, even for two-body problem on a junction, see for instance [16]. Luckily, taking into account the multi-particle interaction does not change essentially the structure of the band spectrum, though some new branches may appear. Based on above motivation we focus in this paper only on one-particle spectral problems on quantum networks. Most interesting are so-called scattering problems formally arising from comparison of spectral properties of the Schrödinger operator on the quantum network and on an unperturbed analog obtained by splitting away the vertex domains, by applying zero boundary conditions on the bottom sections $\Gamma$ of the wires. Unfortunately this splitting and the corresponding matching re-instoring the connection between the wires and the vertex domain. are infinite-dimensional on the bottom sections $\Gamma$. Hence the elegant Glazman theory, see [18], which is very efficient in 1-D case, cannot be applied in the 2D case where we are studying spectral properties of a Hamiltonian of the quantum system composed of several weakly connected blocks. Indeed, the main tool of the theory - von Neumann's operator extension - is efficient only in the case when the weak connection is finite-dimensional. Note that in 1-D networks the matching condition is imposed on 0-D sections, and hence is finite-dimensional. This is actually an attractive feature and a main motivation of numerous papers on 1-D Quantum Networks in the last two decades, including the papers quoted above.

As we have said, in this paper we consider mainly in the 2-D (or, potentially, even higher dimensional) environment and focus on the problems of resonance scattering caused by the spectral properties of the relevant Schrödinger operator on the vertex domain. The 1-D features appear as single-mode scattering on the first spectra band in the resulting solvable model, but the multi-mode scattering remains within reach of our analysis. This comes at the cost of having to assume (realistic) matching conditions on the bottom sections of the scattering Ansatz in the wires to the solution of the Schrödinger equation on the vertex domain, as opposed to quite general considerations. We organize these matching conditions around our version of the Dirichlet-to-Neumann map, introduced in [21], and developed in later publications, see [26–29]. The corresponding matching on the bottom sections is finite-dimensional, but still allows us to observe the transformation of the discrete spectrum of the Schrödinger operator on the vertex domain into the resonance features of the relevant scattering problem.

It is in fact this transformation which defines one of main difficulties in the analysis of a general resonance scattering system and is caused by the eigenvalues of the compact subsystem, embedded into the continuous spectrum of the reservoir weakly connected to it. From a naive point of view, the weak connection may be taken into account by a standard analytic perturbation procedure. Indeed, for a selfadjoint operator $A_0$ in the Hilbert space $E$, *with discrete spectrum*, and the small self-adjoint perturbation $\varepsilon V$, $\| \varepsilon V \| \leqslant \varepsilon$, defines, for each simple isolated eigenvalue $\lambda_s^0$ of $A_0$

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

a branch of eigenvalues $\lambda_s^\varepsilon$ of the perturbed operator $A_\varepsilon := A_0 + \varepsilon V$ represented by a geometrically convergent series

$$\lambda_s^\varepsilon = \lambda_s^0 + \varepsilon\, \lambda_s^0(1) + \varepsilon^2\, \lambda_s^0(2) + \varepsilon^3\, \lambda_s^0(3) + \dots,$$

and the corresponding branch of eigenfunctions, see [17].

Unfortunately, this standard analytic perturbation approach is not efficient for the case of dense discrete spectrum, where the spacing $\rho$ is small. It is also not applicable, generally, to operators with eigenvalues embedded in the continuous spectrum, where the"spacing" $\rho$ vanishes. But this is precisely the case of a quantum Network with infinite wires.

Interestingly, the development of radio-location during WWII met a similar difficulty in the analysis of scattering problems on networks of electromagnetic wave guides, in particular on junctions. The scattering on the junction is a typical perturbation problem for operators with embedded eigenvalues. The perturbation of the problem with embedded eigenvalues causes the transformation of real eigenvalues on the vertex domain of the junction into complex resonances, which can't be easily embedded into the framework of selfadjoint operators. An elegant realization of this program was proposed by P. Lax and R. Phillips, see [30] for equations of second order in time, such as the wave equation. However not for the Schrödinger equation.

Luckily this obstacle can be mended by transferring to the stationary spectral problem, but again the main obstacle arising from the embedded eigenvalues is unavoidable.

To escape the difficulties caused by small or zero spacing in the case of operators with continuous (or dense discrete) spectrum, one may hope to substitute the unperturbed Hamiltonian $A_0$ 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-step procedure $A_0 \to A^\varepsilon \to A_\varepsilon$ is a modification of the usual analytic perturbation procedure, and was suggested implicitly by H. Poincare for problems related to celestial mechanics, see [31], and used effectively for the analysis of Coulomb scattering by Murota and Dollard and subsequently in a general form for quantum problems by Prigogine. In fact in 1972 he announced, see [34], importance of the search

of a practical algorithm for the two-step analytic perturbation procedure

$$A_0 \longrightarrow A^\varepsilon \longrightarrow A_\varepsilon$$

implementing the above. This was probably inspired by the recent (at that time) work of Murota and Dollard, [32, 33], Prigogine attempted to find an Intermediate operator $A^\varepsilon$ in the same form, as a function of the unperturbed operator $A^\varepsilon = \Phi(A_0)$. He also wanted to have the above two step analytic perturbation procedure on the whole Hilbert space. The search for 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.

In hindsight we now see that I.Prigogine's proposal, based on the Intermediate Operator $A^\varepsilon$, was very close to success. His idea is commonly used by physicists in the form of an effective Hamiltonian of a complex quantum systems, and, after an essential modification, in [35] for "geometrical integration" in the dynamical problems of classical mechanics. For resonance scattering systems Poincare's idea was implemented as a modified analytic perturbation procedure with a "jump-start" ( or kick-start) based on construction of a zero-range solvable model of the perturbed Hamiltonian, see [36]. The corresponding zero- range solvable model for the Quantum Network was constructed in [37].

In this review we present our findings in resonance scattering on quantum networks, based on the idea of an Intermediate Hamiltonian, which is constructed via imposing a semi-transparent finite-dimensional boundary condition on the bottom section of the semi-infinite wires, attached to the vertex domain of the junction, see §2 below. In §3 we discuss methods of construction of the scattering matrix based on straightforward computing for DN-map and in section 4 we aim on analytic perturbation procedure for a thin junction and observe the dependence of the scattering matrix on the spectral characteristics of the Schrödinger operator on the vertex domain of the junction. In section 5 we suggest a fitted zero-range model of a 2-D junction in the form of a Quantum Graph, equipped with the matrix Schrödinger operator with constant coefficients on the wires and a zero-range potential with an inner structure substituting the vertex domain with the relevant Schrödinger operator on it. The zero-range potential can be fitted such that the corresponding scattering matrix is approximated by the resonance factor of the full scattering matrix of the junction section 5.

The remaining part of the paper is dedicated to analysis of an elementary example of the simplest T-junction. On this example most of technical tools can be applied. In the Appendix we give a brief discussion of the classical matrix Rouche theorem, which plays a basic role in the resonance scattering.

Most of the material of the review, is presented without proofs, which are published in international mathematical and physical journals, see the references in the text. This review plays a dual role, as a bridge joining the mathematical demands of rapidly growing research area of the theoretical and computational nano-electronics with already developed area of spectral theory and boundary problems in modern mathematics, as we see it "from our corner". On the other hand we hope to attract attention of young researchers to this area of the contact of the traditional and well developed area of spectral theory and boundary problems for partial differential equations - with a rapidly growing research of modern solid-state electronics, with it's demand on new mathematical methods to match an advanced technology and new materials (e.g. carbon nano-structures), which may substitute the traditional Silicon-based structures in the nearest future.

We also anticipate a huge role of the fitted zero-range solvable models in quantum engineering, aiming on design and manufacturing of elements of computers of new generation. The fitted solvable zero-range models give most flexible tool of the mathematical modeling,

compared with classical partial differential equations of Quantum Mechanics, because they reveal a straightforward connections between the basic characteristics of materials employed and most important features of the structures designed. In particular we expect that the fitted zero-range solvable models would play an important role in modern solid-state theory, for design of composite structures with prescribed transport properties. In this connection we attract attention of the reader to our version of analysis of periodic multi-dimensional and sandwich structures, characterized by an extraordinary high mobility of electrons and holes, see [38]. Neither straightforward computing, nor the traditional analytic perturbation procedure for the Schrödinger equation would be able to reveal the high mobility features in the periodic multidimensional or sandwich structures which are naturally described by the corresponding zero-range models.

## 2. Scattering matrix via Intermediate DN map

We begin with more detail concerning the physical environment. The electron's dynamic on the quantum network , in particular, electron's scattering, is observed, roughly speaking, only on a spectral interval $\Delta_T$ defined by the temperature $T$. This interval is centered at the Fermi level $E_F$, see [39] and is described, in terms of the scaled spectral parameter $\lambda = 2m^*E\hbar^{-2}$ by the inequality $2m^*\hbar^{-2}\left[F_F - \kappa T\right] < \lambda < 2m^*\hbar^{-2}\left[F_F - \kappa T\right]$. Here $m^*$ is the effective mass of the electron on the network. On the major part of the paper, if the opposite is not stated, we assume that the mass is isotropic, and, the Fermi level lies at the center of the first spectral band $2m^*E_F\hbar^{-2} := \lambda_F = \pi^2\delta^{-2}5/2 + V_\delta$.

In this paper the spin-dependent transport problem for a single electron with an effective mass $m^*$ is studied on a star-shaped quantum network - a junction $\Omega = \Omega_{int} \cup \omega$ - constructed on a surface $\mathbf{S}$ of a semi-conductor of a vertex domain $\Omega_{int}$ (a quantum well, of an arbitrary shape, with piecewise smooth boundary), and a few straight semi-infinite leads $\omega^m,\ \cup_{m=1}^M \omega^m =: \omega$ ( quantum wires, of a constant width $\delta$) attached to $\Omega_{int}$ at the bottom sections $\Gamma^m,\ \cup_{m=1}^M \Gamma^m =: \Gamma$. In strong

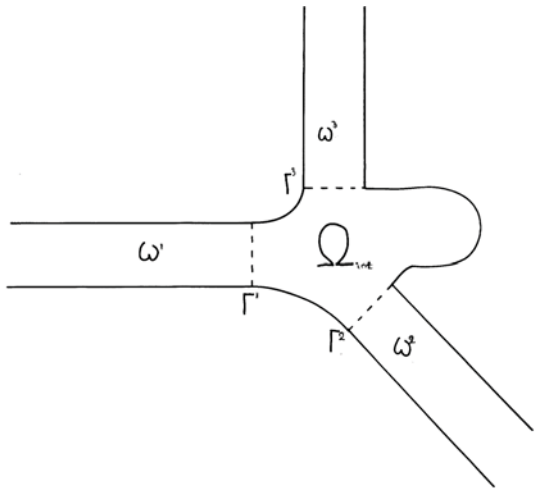


FIG. 2. General T-junction. The bottom sections $\Gamma^s$ of the wires $\omega^s$ are denoted by the stroked lines.

normal electric field the dynamic of the electron on the network is described by the Schrödinger equation which is transformed, after separation of time and scaling of energy $E \to \lambda = 2m^*E\hbar^{-2}$, to the spectral problem on $\Omega$ for the Schrödinger operator

$$\mathcal{L}\psi = -\triangle\psi + H_R\psi + \mathrm{V}_{\ \delta}\psi = \lambda\psi,$$

on 2-spinor $\psi$, with the spin-orbital interaction defined the symmetrized Rashba term:

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

containing the Rashba - factor $\alpha$, see [40], defined by the magnitude of the normal component of electric field. Hereafter we assume, that the normal component of the electric field and the corresponding factor $\alpha$ vanish near the boundary $\partial\Omega_{int}$ and on the wires. Thus the spin-orbital interaction is present on the vertex domain of the junction, but it is switched off on the wires.

We assume that the temperature is low and the Fermi level $\Lambda = 2m^* E_F \hbar^{-2}$ lies deep enough compared to the potential on the surface $\mathbf{S}$ of the semiconductor outside $\Omega$, to assume that $\psi$ vanishes on the boundary of the network. The electrostatic potential $V_{delta}$ is real and piecewise continuous on the network and is constant, $V_\delta = V_\infty$, on the wires, magnetic field is absent. We consider also the Schrödinger equation $L\psi = \lambda\psi$, on the quantum well $\Omega_{in}$ with $L$ defined by the same potential and Rashba term as in $\mathcal{L}$. We consider the selfadjoint operators $L^D, L^N$ in $L_2(\Omega_{in})$, with Dirichlet and Neumann boundary conditions on $\Gamma$ and Dirichlet boundary condition on the remaining part of the piecewise smooth boundary $\partial\Omega_{int}\backslash\Gamma$. These operators as well as the one-electron Hamiltonians $\mathcal{L}$ , are selfadjoint in the Hilbert spaces $L_2(\Omega_{in}), L_2(\Omega)$ of all square-integrable functions on the $\Omega_{in}, \Omega$, on the domain consisting of $W_2^2 \cap W_2^1$ in $\Omega, \Omega_{in}$ respectively, satisfying the above boundary conditions, see [26].

The spectrum of $L^D, L^N$ in $L_2(\Omega_{in})$ is discrete, and the spectrum of $\mathcal{L}$ contains an absolutely-continuous part, see [26]. Transport properties of the junction are defined by the structure of the eigenfunctions of continuous spectrum of $\mathcal{L}$ - scattered waves, see below. The continuous spectrum of the Schrödinger operator $\mathcal{L}$ on the junction, see [26], consists of a countable number of spectral branches $[\pi^2\, l^2\, \delta^{-2} + V_\infty)$, and has constant multiplicity on each spectral band $[\pi^2\, l^2\, \delta^{-2} + V_\delta,\ \pi^2\, (l+1)^2\, \delta^{-2} + V_\infty \equiv \Delta_l]$, increasing at each threshold $\pi^2\, l^2\, \delta^{-2} + V_\delta$ by a standard jump equal to the total number M of the wires attached to the vertex domain. If the Fermi level is situated at the center of the first spectral band, the temperature interval $\Delta_T$ is situated , for low temperature T, on the first spectral band, hence the first branch $[\pi^2\delta^{-2} + V_\infty,\ \infty)$ of the continuous spectrum is an open channel for the scattering dynamic , and all other branches are closed. Then we need the scattered waves only on the first spectral branch. We can construct them based on the cross-section spinors $e_m(y) = \sqrt{2/\delta}\sin\pi y l\delta^{-1}\ \nu_m,\ m = 1, 2 \ldots M$ with $l = 1$. Hereafter we use the coordinates $x^{\|}, x^{\perp}$ along and across the wires, $\omega^m = (x : 0 < x^{\|} < \infty,\ 0 < x^{\perp} < \delta)$. Denote by $E_+ := \bigvee_m \sin\pi x^{\perp}\delta^{-1}\ \nu_m$ the cross-section subspace of the spinors in the open channel in the wires, and by $E_- = L_2(\Gamma) \ominus E_+$ its orthogonal complement in the Hilbert space $L_2(\Gamma)$ of all square integrable functions on the bottom sections of the wires, $\Gamma = \cup_m \Gamma^m$. Hereafter we call $E_+$, $E_-$ the entrance subspaces of the open and closed channels respectively. The scattered waves are constructed via matching on $\Gamma$ of solutions of the Schrödinger equation $L\psi = \lambda\psi$ in $\Omega_{int}$ with the scattering Ansatz $\vec{\psi}(x, \lambda) = \{\psi_l^m(x, \lambda)\}$ in the wires. Generally, for arbitrary position of the Fermi level $\Lambda_F$, the scattering Ansatz is combined of oscillating modes , with $l : \pi^2 l^2 \delta^{-2} + V_\infty < \Lambda_F$, and evanescent modes modes , with $l : \pi^2 l^2 \delta^{-2} + V_\infty > \Lambda_F$ in the wires with exponential behavior at infinity:

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

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

spanned by the cross-section eigen-spinors $e_l(x^{\perp}) = \sqrt{2/\delta} e^l \sin\pi l x^{\perp}\delta^{-1}, l = 1, 2, \ldots$:

$$\psi_l^m(x) = \left\{ \begin{array}{ccc} \chi_+^l(x) + \sum_{\pi^2 r^2/\delta^2 < \lambda} S_{l,r}^{m,m} \chi_-^r(x) & + & \sum_{\pi^2 r^2/\delta^2 > \lambda} s_{l,r}^{m,m} \xi^r(x), x \in \omega^m \\ \sum_{\pi^2 r^2/\delta^2 < \lambda} S_{l,r}^{m,n} \chi_-^r(x) & + & \sum_{\pi^2 r^2/\delta^2 > \lambda} s_{l,r}^{n,m} \xi^r(x), x \in \omega^n,\ n \neq m. \end{array} \right. \quad (1)$$

The quantum wells and the quantum wires are usually manufactured as a certain relief on the surface $\mathbf{S}$ of the semiconductor.

If the scaled Fermi level $\Lambda_F = 2m^*E_F\hbar^{-2}$ is situated inside the first spectral band $\Delta_1 = [V_\infty + \frac{\pi^2}{\delta^2}, V_\infty + 4\frac{\pi^2}{\delta^2}]$ of the wires ( for instance, in the middle of it $\Lambda_F \equiv \Lambda = V_\infty + \frac{5}{2}\frac{\pi^2}{\delta^2}$) then $\Delta_1$ plays the role of the conductivity band in the wires and the junction has metallic properties. We assume additionally the temperature $T$ so low, that the scattering processes are observed only on the essential spectral interval

$$\Delta_T = [\Lambda - 2m^*\kappa T\hbar^2, \Lambda - 2m^*\kappa T\hbar^2] \subset \Delta_1, \tag{2}$$

which is situated entirely inside the first spectral band. If the electron's density is low, the main contribution to the scattering picture is defined by one-body processes. 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 $L_2(\Gamma) =: E$ as an orthogonal sum of the entrance subspaces $E_\pm$ of the open and closed spectral channels respectively:

$$E_+ \;=\; \bigvee_{m=1}^{M} e_1^m, \quad E_- \;=\; \bigvee_{m=1}^{M}\bigvee_{l=2}^{\infty} e_l^m, \quad P_{E_\pm} =: P_\pm. \tag{3}$$

The infinite linear system for the coefficients of the scattering Ansatz, obtained from the matching conditions, can be solved, if the Green functions $G^D_{\Omega_{int}} \equiv G_{int}$ of the Schrödinger operators $L^D_{Omega_{int}} \equiv L^D_{int}$ in $L_2(\Omega_{int})$, with Dirichlet boundary conditions is constructed. The operator $L^D_{int}$ is defined on $W_2^2$-functions in $\Omega_{int}$, with the Meixner conditions, $u \in W_2^2 \cap W_2^1$ which allow only limited singularity at the inner corner points:

$$L^D_{int}u = -\Delta u + Vu = \lambda u,\ u\big|_{\partial\Omega_\int} = 0. \tag{4}$$

The Green function is found from the equation:

$$L^D_{int}G^D_{int} \;=\; -\triangle G^D_{int} + VG^D_{int} \;=\; \lambda G^D_{int} + \delta(x-y),\ G^D_{int}\big|_{\partial\Omega_{int}} \;=\; 0. \tag{5}$$

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

$$-\Delta u + Vu = \lambda u,\ u\big|_\Gamma = u_\Gamma,\ u\big|_{\partial\Omega_\int\setminus\Gamma} = 0. \tag{6}$$

is represented by the Poisson map

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

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

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

This formal integral operator is the restriction onto $\Gamma$ of the Dirichlet-to-Neumann map, see [41–43] and denote as $\mathcal{DN}_\Gamma$. For the sake of brevity we call it here "relative DN-map". The relative DN- map is a Nevanlinna class function $\mathcal{DN}_\Gamma(\lambda) > 0$ for Im $\lambda \leqslant 0$, with poles at the eigenvalues of the corresponding Schrödinger operator $L^D_{\Omega_{int}} = L^D_{int}$. For the vertex domain with a smooth boundary the relative DN–map is a pseudo–differential operator of order 1: for $W_2^2(\Omega)$ solutions $u$ the DN–map acts from $W_2^{3/2}(\Gamma)$ to $W_2^{1/2}(\Gamma)$ and for $W_2^{3/2}(\Omega)$ generalized solutions the D–map acts from $W_2^1(\Gamma)$ to $L_2(\Gamma)$.

We consider also the boundary problem

$$-\Delta u + Vu = \lambda u,\ \frac{\partial u}{\partial n}\big|_\Gamma = \rho_\Gamma,\ u\big|_{\partial\Omega_\int\setminus\Gamma} = 0. \tag{7}$$

and the operator

$$L^N_\Gamma = -\Delta u + Vu,\ \frac{\partial u}{\partial n}\big|_\Gamma = 0,\ u\big|_{\partial\Omega_\int\setminus\Gamma} = 0. \tag{8}$$

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

$$L^N_\Omega G^N_\Omega \ = \ -\triangle G^N_\Omega + VG^N_\Omega \ = \ \lambda G^N_\Omega + \delta(x-y),\ G^N_\Omega\big|_{\partial\Omega_{int}\setminus\Gamma} \ = \ 0,\ \frac{\partial G^N}{\partial n_x}\big|_\Gamma = 0. \tag{9}$$

The map

$$u(x) \ = \ \int_\Gamma G^N_\Omega(x,\gamma,\lambda)\rho_\Gamma(\gamma)d\ \Gamma \ =: Q^\Omega_1\rho_\Gamma, \quad x\in\Omega_{int}\ ,$$

gives a solution of the relative Neumann boundary problem.

$$L^N_{int}u \ = \ -\triangle u + Vu \ = \ \lambda u,\ u\big|_{\partial\Omega_{int}\setminus\Gamma} \ = \ 0,\ \frac{\partial u}{\partial n_x}\big|_\Gamma = \rho_\Gamma. \tag{10}$$

The trace of the solution on $\Gamma$

$$u(x)\big|_\Gamma \ = \ \int_\Gamma G^N_{int}(x,\gamma)\rho_\Gamma d\ \Gamma \ =: \mathcal{N}\mathcal{D}_\Gamma\frac{\partial\psi}{\partial n}\Big|_\Gamma,\ x\in\Gamma\ ,$$

defines the relative Neumann–to–Dirichlet map $\mathcal{N}\mathcal{D}_\Gamma$ which is inverse to the relative Dirichlet–to–Neumann map defined above,

$$\mathcal{N}\mathcal{D}_\Gamma\ \mathcal{D}\mathcal{N}_\Gamma \ = \ I_\Gamma.$$

For $W^2_2$ solutions $u$ of the above Schrödinger equation in $\Omega_{int}$ with the smooth boundary 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 $W^1_2(\Gamma)$. Hereafter we omit the lower index $\Gamma$ on the $\mathcal{D}\mathcal{N}_\Gamma, \mathcal{N}\mathcal{D}_\Gamma$ notations

$$\mathcal{D}\mathcal{N}_\Gamma \equiv \mathcal{D}\mathcal{N},\ \mathcal{N}\mathcal{D}_\Gamma \equiv \mathcal{N}\mathcal{D}.$$

The coefficients of the scattering Ansatz (1) can be found, in principle, from the infinite linear system which is obtained by substitution of the scattering Ansatz into the matching condition (see [26]). An important part of the calculation is the proof of the formula for the DN–map in terms of the $G^D_\Omega$ (see [26]), or, respectively, a similar formula for the ND–map in terms of $G^N_\Gamma$. Selecting $E_\pm$ as indicated above, (3), represent the ND–map of $L^N_\Omega \equiv L^N_{int}$ by $2\times 2$ operator matrix with elements $\mathcal{N}\mathcal{D}_{\pm,\pm} \equiv \ P_\pm\mathcal{N}\mathcal{D}_\Gamma P_\pm$

$$\mathcal{N}\mathcal{D}_\Gamma = \begin{pmatrix} \mathcal{N}\mathcal{D}_{++} & \mathcal{N}\mathcal{D}_{+-} \\ \mathcal{N}\mathcal{D}_{-+} & \mathcal{N}\mathcal{D}_{--} \end{pmatrix}. \tag{11}$$

A similar decomposition of the DN–map of the Schrödinger operator $L^D_\Gamma$ on $\Omega_{int}$

$$\mathcal{D}\mathcal{N}_\Gamma \ = \ \begin{pmatrix} \mathcal{D}\mathcal{N}_{++} & \mathcal{D}\mathcal{N}_{+-} \\ \mathcal{D}\mathcal{N}_{-+} & \mathcal{D}\mathcal{N}_{--} \end{pmatrix} \tag{12}$$

was used in [26] in the course of construction of a convenient representation for the scattering matrix on the open spectral bands. Denoting the thresholds $\pi^2 l^2 d^{-2} \equiv \lambda_l,\ l = 1,2,\ldots$, we introduce the exponents of the modes in the open and close channels:

$$\begin{aligned} K_+ \ &= \ \textstyle\sum_m\sum_{open}\sqrt{\lambda-\lambda_l}\,e^m_l\rangle\langle e^m_l \ = \ \sum_m\sqrt{\lambda-\frac{\pi^2}{\delta^2}}\,e^m_1\rangle\langle e^m_1\ , \\ K_- \ &= \ \textstyle\sum_m\sum_{closed}\sqrt{\lambda_l-\lambda}\,e^m_l\rangle\langle e^m_l \ = \ \sum_m\sum_{l\geqslant 2}\sqrt{\lambda_l-\lambda}\,e^m_l\rangle\langle e^m_l\ . \end{aligned} \tag{13}$$

Hereafter we use the standard bra/ket notations, $e >< e'\ u \to e\ < e', u >$, 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:

$$\chi_\pm e_+ = e^{\pm iK_+ x} e_+ \ , \qquad \xi_- e_- = e^{-K_- x} e_- \ .$$

The matrices $S^{m,n}_{l,r}$ and $s^{m,n}_{l,r}$, 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 ($l = 1$):

$$S = \sum_{m,n=1}^{M} \ \sum S^{m,n}_{1,1} e^m_1 \rangle \ \langle e^n_1 \ ,$$

and the table of amplitudes in front of the evanescent modes

$$s \ = \ \sum_{m,n=1}^{M} \ \sum_{1,\, r \geqslant 2} s^{m,n}_{1,r} e^m_1 \rangle \ \langle e^n_r \ .$$

With above notations introduced, the Ansatz (1) for the scattered wave iniciated by the plain wave, incoming from $\infty$ with the cross-section spinor $e \in E_+$, can be represented as

$$\Psi_e = e^{iK_+ x} e + e^{-iK_+ x} S e + e^{-K_- x} s e. \tag{14}$$

Inserting this Ansatz formally into the boundary condition at the bottom section $\Gamma$, we can obtain an explicit expression for the scattering matrix in terms of matrix elements $\mathcal{DN}$, $\mathcal{ND}$ combined into the aggregates

$$\mathcal{M} \ = \ \mathcal{DN}_{++} - \mathcal{DN}_{+-} \frac{I}{\mathcal{DN}_{--} + K_-} \mathcal{DN}_{-+} \tag{15}$$

$$\mathcal{N} \ = \ \mathcal{ND}_{++} - \mathcal{ND}_{+-} K_- \frac{I}{I_- + \mathcal{ND}_{--} K_-} \mathcal{ND}_{-+} \ , \tag{16}$$

see the Theorem 2.1 below. To calculate the aggregates we need to verify the existence of the inverse of the denominators

$$[\mathcal{DN}_{--} + K_-] \equiv \mathcal{D}^D, \ [I_- + \mathcal{ND}_{--} K_-] \equiv \mathcal{D}^N,$$

on the major part of the conductance spectral band. 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:

$$\frac{\pi^2 (l+1)^2}{\delta^2} - \frac{\pi^2 l^2}{\delta^2} \ = \ \frac{(2l+1)\pi^2}{\delta^2} \ .$$

It is noticed in [26] that, for a "thin junction", the denominator $\mathcal{DN}_{--} + K_-$ is invertible on a major part of a properly selected essential spectral interval $\Delta_T$, where the DN-map is represented as a sum of a rational function and a regular correcting term:

$$\mathcal{DN} = \sum_{\lambda_s \in \Delta} \frac{\frac{\partial \varphi_s}{\partial n} \rangle \langle \frac{\partial \varphi_s}{\partial n}}{\lambda_s - \lambda} + \mathcal{K}^{\Delta_1} =: \mathcal{DN}^\Delta + \mathcal{K}^\Delta, \tag{17}$$

The zeros of the denominator $\mathcal{DN}_{--} + K_-$ on $\Delta_T$ have an important operator–theoretic meaning: they are eigenvalues of the *Intermediate Hamiltonian*, see [21, 26] and a discussion in Appendix 2. Hereafter we consider the rational approximation (17) and the corresponding rational approximation of $\mathcal{DN}_{--} = P_- \mathcal{DN} P_-$:

$$\mathcal{DN}_{--} = \mathcal{DN}^\Delta_{--} + \mathcal{K}^\Delta_{--}, \tag{18}$$

with a regular "error" $\mathcal{K}_{--}^{\Delta}$ on a complex neighborhood $G(\Delta)$ of the essential spectral interval $\Delta_T$.

**Definition 2.1.** *We call the junction $\Omega$ thin in closed channels on $\Delta_T$ if $\mathcal{K}_{--}^{\Delta} + K_-$ is invertible on $\Delta_T$.*

This is true if, in particular, if $K_-$ dominates $\mathcal{K}_{--}^{\Delta}$ either in $W_2^1(\Gamma)$ or in $W_2^{3/2}(\Gamma)$

$$\sup_{\Delta} \parallel K_-^{-1}\mathcal{K}_{--}^{\Delta} \parallel_{W_2^1(\Gamma)} < 1 \ , \qquad \text{or} \qquad \sup_{\Delta} \parallel K_-^{-1}\mathcal{K}_{--}^{\Delta} \parallel_{W_2^{3/2}(\Gamma)} < 1 \tag{19}$$

We will use the following test for the invertibility of the denominator $\mathcal{D}^D$ in 15(see [26]):

**Lemma 2.1.** *If the junction is thin in closed channels, $\Delta_T$, then the denominator $K_- + \mathcal{D}\mathcal{N}_{--}^{\Delta}(\lambda) \equiv \mathcal{D}$ of the intermediate DN- map is invertible on the corresponding "major part of the essential spectral interval" - the complement of the sufficiently small, depending on $\mathcal{K}_{--}^{\Delta}$, $K_-$, neighborhood set of zeros $Z_\Delta \subset \Delta$ of the determinant of the finite-dimensional matrix-function :*

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

*The zeros of the denominator are the eigenvalues of the Intermediate Hamiltonian $L_{int}^D$.*

**Theorem 2.1.** *The substitution of the scattering Ansatz (1) into the matching conditions on $\Gamma$ gives the following formula for the scattering matrix on $\hat{\Delta}$*

$$S = \left[ iK_+ + \mathcal{M} \right]^{-1} \left[ iK_+ - \mathcal{M} \right] \ , \tag{20}$$

$$S = \left[ \mathcal{N}iK_+ + 1 \right]^{-1} \left[ \mathcal{N}iK_+ - 1 \right] \ . \tag{21}$$

*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 $\Omega_{int}$:

$$L_{int}\psi \ = \ \lambda\psi, \qquad \psi\Big|_{\partial\Omega_{int}\setminus\Gamma} \ = \ 0 \ ,$$

$$\psi\big|_\Gamma = \psi_e(0) = e + Se + se \ , \qquad \frac{\partial\psi}{\partial n}\bigg|_\Gamma \ = \ \psi_e'(0) \ = \ iK_+e - iK_+Se - K_-se \ . \tag{22}$$

Using the matrix representations (12 and 11) for $\mathcal{D}\mathcal{N}$, $\mathcal{N}\mathcal{D}$, we obtain from (22) two equivalent linear systems which describe matching conditions on $\Gamma$

$$\begin{aligned} iK_+(1-S)e \ &= \ \mathcal{D}\mathcal{N}_{++}(1+S)e + \mathcal{D}\mathcal{N}_{+-}se \ , \\ -K_-se \ &= \ \mathcal{D}\mathcal{N}_{-+}(1+S)e + \mathcal{D}\mathcal{N}_{--}se \ , \end{aligned} \tag{23}$$

and

$$\begin{aligned} (I+S)e \ &= \ \mathcal{N}\mathcal{D}_{++}\, i\, K_+(I-S)e - \mathcal{N}\mathcal{D}_{+-}K_-se, \\ [I + \mathcal{N}\mathcal{D}_{--}K_-]se \ &= \ \mathcal{N}\mathcal{D}_{-+}\, i\, K_+(I-S)e\mathcal{N}\mathcal{D}_{--}se. \end{aligned} \tag{24}$$

Eliminating the component $se$ from them and using the former notations $\mathcal{M}$, $\mathcal{N}$ we obtain the announced representation for the scattering matrix (20,21).

*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 $\partial\Omega$. It is essentially

self–adjoint on the domain of smooth functions $u$, subject to the Meixner restriction $u \in W_2^1(\Omega)$. 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:

$$P_+ u\big|_\Gamma \;=\; 0\;, \tag{25}$$

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:

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

Here $l^0 = -\dfrac{d^2}{dx^2} + \frac{\pi^2}{\delta^2} + V_\delta$ in $L^2(0,\infty)\times E_+) =: \mathcal{H}_+$, with zero boundary condition at the origin $u(0) = 0$, and $L^0$ is defined in the orthogonal sum of the channel space $L^2(0,\infty)\times E_- =: \mathcal{H}_-$ of the closed channels and $L_2(\Omega_{int})$ on $W_2^2$ - smooth functions, subject to the Meixner condition and the matching condition on $\Gamma$ in closed channels:

$$L_\Lambda : D(_\Lambda) \;\longrightarrow\; L_2(\Omega_{int}) \oplus \mathcal{H}_-\;.$$

**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*

$$\begin{aligned} \sigma_a(l_\Lambda) \;&=\; [\lambda_1,\,\infty), \qquad \textit{with multiplicity } M,\\ \sigma_a(L_\Lambda) \;&=\; \bigcup_{l=2}^{\infty}[\lambda_l,\infty) \;=: \bigcup_{l\geqslant 1}\sigma_a^l\;. \end{aligned} \tag{26}$$

*where each branch $\sigma_a^l$ has multiplicity $M$, and the total multiplicity is growing stepwise 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 $Ml(l+1)/2$. The discrete spectrum of $L_\Lambda$ consists of a countable set of eigenvalues $\lambda_s^\Lambda$ accumulating at infinity. The singular spectrum of $L^0$ is empty.*

The relation $\mathcal{M}\mathcal{N} = I$ observed from comparison of the formulae (21), (20) 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

$$\mathcal{L} \longrightarrow \mathcal{L}_\Lambda \;=\; L_\Lambda \oplus l_\Lambda. \tag{27}$$

defined by the partial boundary condition $P_+ u\big|_\Gamma = 0$. Contrary to the standard splitting $\mathcal{L} \longrightarrow L_{int} \oplus L^\omega$, this splitting (27) is finite–dimensional — see [18]. The poles of $\mathcal{M}$ on the first spectral band, below $\lambda_{min}$, are the eigenvalues of $L_\Lambda$.

### 2.1. Boundary conditions at the vertex

The formula (15) gives a practical algorithm of calculation of the scattering matrix based on energy-dependent boundary condition on the scope $\Gamma$ of all bottom sections adjacent to the given vertex domain $\Omega_{int}$: the scattering matrix is obtained via matching the solution $\Psi(x,p)$ of the Schrödinger equation in the open channels of the wires

$$-\frac{d^2\Psi}{dx^2} + K_+^2\Psi = \lambda\Psi$$

satisfying the boundary condition at the bottom section

$$\left.\frac{dPsi}{dx}\right|_\Gamma = \mathcal{M}(\lambda)\Psi\;\Big|_\Gamma.$$

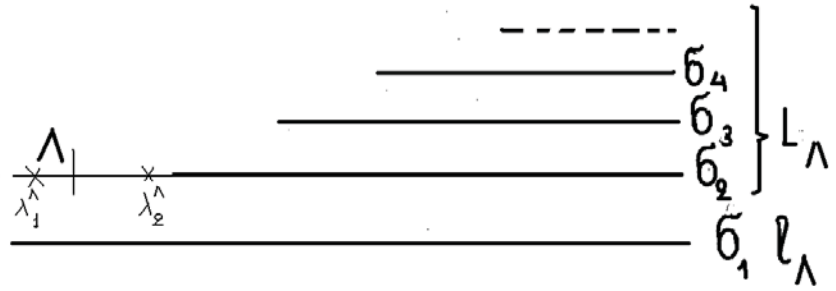


FIG. 3. The intermediate Hamiltonian $L_\Lambda$ inherits the closed branches of the continuous spectrum of the unperturbed operator. The part $l_\Lambda$ of the split operator inherits the first - open - branch of the spectrum of the split operator. The resonance eigenvalues of the intermediate Hamiltonian define the resonance conductance of the junction

It may provoke the reader to follow the classical idea of E. Wigner, see [19], to substitute a compactly supported potential of the Schrödinger operator in the scattering problem by the corresponding energy-dependent boundary condition on a sphere of a ball containing the support of the potential, and then find the scattering matrix from the boundary condition bearing the information on the inner problem on the ball- the Dirichle -to- Neumann map of the corresponding Schrödinger operator on the ball. Unfortunately the price to pay for this simplified approach to the scattering problem is too high: though formally the above spectral problem with an energy-dependent boundary condition allows to calculate the scattering problem, yet the basic laws of quantum mechanics are violated: the problem with the energy dependent boundary condition does not depend a selfadjoint operator, hence, just formally, we can't define a natural quantum dynamics based on it. and hence can't use it for mathematical modeling of quantum processes. Nevertheless the temptation to calculate the scattering matrix based on above energy-dependent boundary condition is too high, and, fortunately, the energy dependence may be, to some extent ignored. Indeed, consider the 1-D star-graph with $n$ rays outgoing from the vertex point $\vec{x} = 0$, with the Schrödinger operator $l = -\frac{d^2}{dx^2}$ on it. Integration by parts with smooth functions $u, v$ permits to calculate the boundary form:

$$J(\vec{u}, \vec{u}) = \langle l\vec{u}, \vec{v}\rangle - \langle \vec{u}, l\vec{u}\rangle = \sum_{m=1}^{N} [\bar{u}'_m v_m - \bar{u}_m v'_m]. \tag{28}$$

Probably the simplest nontrivial family of hermitian boundary condition can be parametrized by complex $N$ - vectors $\vec{\beta}$ in the following form:

$$\vec{u}' \parallel \vec{\beta},\ \vec{u} \perp \vec{\beta},\ \text{or}\quad \vec{u} \parallel \vec{\beta},\ \vec{u}' \perp \vec{\beta}. \tag{29}$$

This boundary condition was proposed in [59], with the vector $\vec{\beta} = (1, \beta, 1)$, as a detail of a simplest solvable model of a symmetric T - junction, and soon became popular in practical design of simplest junctions, see [60, 61]. Physical meaning of the phenomenological parameter $\vec{\beta}$ was

interpreted in [27], for low temperatures and thin junctions, in terms of a resonance eigenfunction on the corresponding vertex domain. Here is a sketch of the corresponding reasoning.

It is known that the scattering processes are observed for energy close to Fermi-level, $\Lambda - \frac{2m*\kappa T}{\hbar^2} < \lambda < \Lambda + \frac{2m*\kappa T}{\hbar^2}$. Assume that there is a simple eigenvalue of the Intermediate Hamiltonian $L^\Lambda$, which coincides with the Fermi level, $\lambda_1 = \Lambda$, and the corresponding eigenfunction of the Intermediate Hamiltonian is $\psi$, so that the Intermediate DN-map admits the rational approximation $\mathcal{DN}_\Lambda = \frac{\frac{\partial\psi_1}{\partial n}(\gamma)\rangle\,\langle\frac{\partial\psi_1}{\partial n}(\gamma')}{\lambda-\lambda_1} + \mathcal{K}(\gamma,\,\gamma')$, with an hermitian integral operator $\mathcal{K}$. If the Fermi level is situated on the first spectral band $\frac{\pi^2}{\delta^2} + V_{infty} < \Lambda < 4\frac{\pi^2}{\delta^2} + V_{infty}$, $\Lambda \approx \frac{5}{2}\frac{\pi^2}{\delta^2} + V_{infty}$, and the residue of the polar term of the DN-map at $\lambda_1$ is

$$\frac{\partial\psi_1}{\partial n}(\gamma)\rangle\,\langle\frac{\partial\psi_1}{\partial n}(\gamma') = d\nu\rangle\,\langle\nu' \equiv dP_1,$$

then, with $P_1 = \nu\rangle\,\langle\nu'$ we have, the rational approximation for the intermediate DN-map on the essential spectral interval $\Delta = \left[\Lambda - \frac{2m*\kappa T}{\hbar^2},\, \Lambda + \frac{2m*\kappa T}{\hbar^2}\right]$ $\mathcal{DN}(\lambda) = dP_1 + \mathcal{K}$, and an asymptotic for the scattering matrix $S(p)$, for the resonance values of momentum $p$, $p^2 = \lambda - \left[\frac{\pi^2}{\delta^2} + V_{infty}\right] \approx \Lambda - \left[\frac{\pi^2}{\delta^2} + V_{infty}\right] = p_1^2 \approx \frac{3}{2}\,\frac{\pi^2}{\delta^2}$dominating $\mathcal{K}$:

$$S(p) \approx \frac{ip + d\frac{P_1}{p_1^2-p^2}}{ip - d\frac{P_1}{p_1^2-p^2}} \approx P_1^\perp + \frac{[p - p_1 + id(2p_1^2)^{-1}]\,[p + p_1 + id(2p_1^2)^{-1}]}{[p - p_1 - id(2p_1^2)^{-1}]\,[p + p_1 - id(2p_1^2)^{-1}]}P_1. \tag{30}$$

This asymptotic corresponds to the relevant asymptotic for the intermediate DN-map:

$$\mathcal{DN}_\Lambda = \frac{d\;\;P_1}{p^2 - p_1^2}, \text{with}\;\; P_1 = \nu\rangle\,\langle\nu \tag{31}$$

or the boundary condition

$$\left.\frac{\partial u}{\partial n}\right|_\Gamma = \frac{dP_1}{p^2 - p_1^2}\;\left.u\right|_\Gamma : \left.\frac{\partial u}{\partial n}\right|_\Gamma \approx \nu. \tag{32}$$

Then $d(p^2 - p_1^2)\;\left.\frac{\partial u}{\partial n}\right|_\Gamma = P_1 u\Big|_\Gamma$ implies, for zero temperature, $(p^2 - p_1^2)\;\;\left.P_1 u\right|_\Gamma = 0$. Comparison of (30,32) with (29) allows to interpret the phenomenological parameter $\vec{\beta} = \nu$.The scattering matrix recovered from the model $S \approx P_\perp - P_1$ does not depend on the spectral parameter, but is unitary and gives a reasonable first-step approximation for low temperature. Similar reasoning with ND - map gives an interpretation for the second boundary condition in the pair (29).

## 3. Direct computing with the intermediate Hamiltonian

The importance of direct calculation of the Dirichlet-to-Neumann map of a vertex domain for the spectral analysis of the Laplacian on a manifold with cusps was noticed in [9, 12, 13]. Based on these observations Levitin, see [14] proposed a formal algorithm for the calculation of the DN-map of a Laplacian on a compact domain $\Omega_{int}$ in terms of the bi-linear form of the Laplacian with respect to a basis of solutions of boundary problems with the boundary data defined by corresponding basis in $L_2(\partial\Omega_{int})$.

Our approach here to the one-body scattering problem is based on the Intermediate Hamiltonian $L_\Lambda$ which is defined as a selfadjoint operator on the orthogonal complement of the open channels $L_2(R_+) \times E_+$, with the boundary condition on the inner and exterior sides

$\Gamma_{int}$, $\Gamma_{ext}$ of the bottom sections $\Gamma$ of the wires:

$$P_+u\Big|_{\Gamma} = 0,\ P_-\frac{\partial u}{\partial n}\Big|_{\Gamma_{int}} = P_-\frac{\partial u}{\partial n}\Big|_{\Gamma_{ext}},\ P_-u\Big|_{\Gamma_{int}} = P_-u\Big|_{\Gamma_{ext}}. \tag{33}$$

The matching conditions applied to the boundary values of the Sobolev class solutions of the homogeneous equation $\mathcal{L}$ on $\Omega = \Omega_{int} \cup \omega$ with the spectral parameter from the first spectral band $\Delta_1$, can be substituted by the Robin-type boundary condition at the bottom section,

$$P_-\frac{\partial u}{\partial n}\ \Big|_{\Gamma_{int}} = K_-u\Big|_{\Gamma_{int}},\ P_+u\ \Big|_{\Gamma_{int}} = 0,\ u\ \Big|_{\partial\Omega_{int}\setminus\Gamma_{int}} = 0 \tag{34}$$

because the component of the solution in the wires can be found via separation of variables. The above boundary condition (34) for fixed $\lambda \in \Delta_1$ is selfadjoint, since $K_-(\lambda) > 0$ and hence the restriction of the inverse of the Intermediate Hamiltonian onto $L_2(\Omega_{int})$ is represented, thanks to L. Schwartz's theorem [44], in the form of an integral operator with a kernel $G_\Lambda$, playing the role of the Green function of the restriction of the inverse onto the vertex domain $\Omega_{int}$ of the junction:

$$P_{L_2(\Omega_{int})}\,(L_\Lambda - \lambda I)\ \ f\ \ (x) = \int_{\Omega_{int}} G_\Lambda(x,s)f(s)d\Omega_{int},\ \text{for}\ \ f \in L_2(\Omega_{int}),\ \ x \in \Omega_{int} \tag{35}$$

The Green function $G_\Lambda(x,s)$ pertain the typical 2D logarithmic singularity at the pole $x = s$, and defines the Poisson kernel on the inner side $\Gamma_{int}$ of the bottom section:

$$P_{\Gamma_{int}}(x,s) = -\frac{\partial G_\Lambda}{\partial n_s},\ \ s \in \Gamma_{int},\ \ x \in \Omega_{int}.$$

The component of the Green function in $\Omega_{int}$ can be found as a solution of the inhomogeneous equation

$$-\Delta\psi + H_R\,\psi + V_\delta\,\psi - \lambda\,\psi = \delta(x-s),$$

with the above condition (34) on the boundary.

The algorithm suggested in [14] can be adjusted for calculation of the relative DN-map, the intermediate DN map, and spectral characteristics of the intermediate Hamiltonian. Eventually, we are able to estimate the positions of resonances and the evaluate the resonance states based on the matrix-valued Rouche theorem and the above exact formulas for the scattering matrix, see Theorem 2.1. This bridges the computational and analytical approaches to the scattering problem on the junction.

### 3.1. Calculation of the relative DN-map and ND-map

Let $\{\varphi_n\}, n = 1, 2, \ldots$ be an orthogonal basis in $L_2(\Gamma)$. We consider two relative boundary problems for the Schrödinger equation $Lu = \lambda u$:

$$Lu = \lambda u,\ u\big|_{\Gamma} = \varphi_n,\ u\big|_{\partial\Omega_{int}\setminus\Gamma} = 0, \quad n = 1, 2, \ldots.$$

and

$$Lu = \lambda u,\ \frac{\partial u}{\partial n}\big|_{\Gamma} = \varphi_n,\ u\big|_{\partial\Omega_{int}\setminus\Gamma} = 0, \quad n = 1, 2, \ldots.$$

The boundary problems have unique finite energy solutions in the Sobolev class $W_2^2(\Omega_{int}) \cap W_2^1(\Omega_{int})$ if the spectral parameter $\lambda$ does not lie on the spectrum of the corresponding spectral problem. A straightforward integration by parts with solutions $\Phi_i^D$ of the first, or $\Phi_j^N$ of the second, boundary problem yields

$$\int_\Gamma \frac{\partial\bar\Phi_i^D(\gamma)}{\partial n}\ \Phi_k^D(\gamma)d\Gamma = \int_{\Omega_{int}} \left[\nabla\bar\Phi_i^D(x)\ \nabla\,\Phi_k^D(x) + \left(\bar H_r\,\bar\Phi_i^D(x) + V_\delta\bar\Phi_i^D(x) - \lambda\bar\Phi_i^D(x)\right)\ \Phi_k^D(x)\right] d\Omega_{int}d\Omega \tag{36}$$

and, respectively

$$\int_\Gamma \frac{\partial\bar\Phi_i^N(\gamma)}{\partial n}\ \Phi_k^N(\gamma)d\Gamma = \int_{\Omega_{int}} \left[\nabla\bar\Phi_i^N(x)\ \nabla\,\Phi_k^N(x) + \left(\bar H_r\,\bar\Phi_i^N(x) + V_\delta\bar\Phi_i^N(x) - \lambda\bar\Phi_i^N(x)\right)\ \Phi_k^N(x)\right] d\Omega_{int}d\Omega \tag{37}$$

The former integral is the matrix element of the relative DN-map

$$\int_\Gamma \frac{\partial\bar\Phi_i^D(\gamma)}{\partial n}\ \Phi_k^D(\gamma)d\Gamma = \langle\mathcal{D}\mathcal{N}_\Gamma\varphi_i,\ \varphi_k\rangle_{L_2(\Gamma)}$$

element, and the latter is the matrix of the ND-map:

$$\int_\Gamma \frac{\partial\bar\Phi_i^N(\gamma)}{\partial n}\ \Phi_k^N(\gamma)d\Gamma = \langle\varphi_i,\,\mathcal{N}\mathcal{D}\,\varphi_k\rangle_{L_2(\Gamma)}$$

Due to the uniqueness here for elliptic equations the spectra of the the relative Dirichlet and Neumann problems do not overlap and hence for a given value $\lambda\in\Delta_1$ of the spectral parameter, either the matrix $\mathcal{D}\mathcal{N}$ or $\mathcal{N}\mathcal{D}$ is regular.

### 3.2. Calculation of the intermediate DN-map

The above calculation for the relative DN-map and ND-map can be now effected using fairly standard software. However, the above formulas (20) and (21) for the scattering matrix derived in Theorem 2.1 require the intermediate DN and ND maps. These maps are defined based on solutions of another pair of boundary problems.

Assuming that the entrance subspace $L_2(\Gamma)\equiv E$ of the wires is decomposed as an orthogonal sum $E=E_+\oplus E_-$ of the entrance subspaces of the open and closed channels, we construct the basis in $E$ as an orthogonal sum of bases $\{\varphi_s^+\}\subset E_+$ and $\{\varphi_s^-\}\subset E_-$. These bases can be selected from the eigenfunctions of the Laplacian $-\Delta^\perp$ on the bottom cross-sections $\Gamma$, so that the exponents $K_\pm$ have a diagonal form in the basis. Since the eigenvalues $\lambda_s^\perp$ of the Laplacian $-\Delta^\perp$ serve as thresholds in the exponents, we obtain the spectral representations for the exponents in terms of the projectors $P_s\equiv\varphi_s^-\rangle\,\langle\varphi_s^-$

$$K_+(\lambda)=\sum_{\lambda_s<\Lambda}\sqrt{\lambda-\lambda_s}\,P_s,\ K_-(\lambda)=\sum_{\lambda_s>\Lambda}\sqrt{\lambda-\lambda_s}\,P_s^-,$$

and a similar representations for $P_\pm$: $P_+=\sum_{\lambda_s<\Lambda}P_s^+$, $P_-=\sum_{\lambda_s>\Lambda}P_s^-$.

If the spectral point $\lambda$ is not an eigenvalue of the Intermediate Hamiltonian, then the intermediate boundary problems

$$\mathcal{L}u=\lambda u,\ u\Big|_{\partial\Omega_{int}\setminus\Gamma}=0,\ P_-\left[\frac{\partial u}{\partial n}+K_-u\right]\Big|_\Gamma=0,\ P_+u\Big|_\Gamma=\varphi_s^+, \tag{38}$$

$$\mathcal{L}u=\lambda u,\ u\Big|_{\partial\Omega_{int}\setminus\Gamma}=0,\ P_-\left[\frac{\partial u}{\partial n}+K_-u\right]\Big|_\Gamma=0,\ P_+\frac{\partial u}{\partial n}\Big|_\Gamma=\varphi_s^+. \tag{39}$$

Solutions of the above boundary problems are denoted hereafter as $\Phi^D_{intm,i},\ \Phi^N_{intm,i}$. The bi-linear form of the intermediate DN and ND maps are represented as:

$$\langle \mathcal{DN}_\Lambda \varphi_i^+, \varphi_k^+ \rangle = \langle P_+ \frac{\partial \Phi^D_{intm,i}}{\partial n}\Big|_\Gamma, \varphi_k^+ \rangle$$

$$= \int_{\Omega_{int}} \left[\nabla \bar{\Phi}^D_{intm,i}(x)\ \nabla\, \Phi^D_{intm,k}(x) + \left(\bar{H}_r + V_\delta - \lambda I\right) \bar{\Phi}^D_{intm,i}(x) \Phi^D_{intm,k}(x)\right] d\Omega_{int} \quad (40)$$

$$\langle \varphi_i^+, \mathcal{ND}_\Lambda \varphi_k^+ \rangle = \langle P_+ \frac{\partial \Phi^N_i}{\partial n}\Big|_\Gamma, \Phi^N_{intm,k} \rangle$$

$$= \int_{\Omega_{int}} \left[\nabla \bar{\Phi}^N_{intm,i}(x)\ \nabla\, \Phi^N_{intm,k}(x) + \left(\bar{H}_r + V_\delta - \lambda I\right) \bar{\Phi}^N_{intm,i}(x) \Phi^N_{intm,k}(x)\right] d\Omega_{int}. \quad (41)$$

Hence for each spectral point $\lambda \in \Delta_1$ at least one of the formulas (20) or (21) derived in the Theorem 2.1 can be used as a convenient representation of the scattering matrix.

Unfortunately the boundary problem for the Intermediate Hamiltonian is not standard: there is no commercial software to compute the solution of the problems (38) and (39). One of prime aims of this paper is to attract the attention of specialists in these matters to these important problems.

### 3.3. Straightforward computing for the scattering matrix and resonances

The above non-spectral approach to the calculations of the DN and ND maps permits us to calculate the polar terms of the DN-map and reveal the resonance character of the scattering matrix near the eigenvalues of the intermediate Hamiltonian without a formal solution of the spectral problem.

Assume that the the scaled Fermi level $\Lambda$ is situated within the first spectral band

$$\Lambda \in \Delta_1 = \left[\pi^2\delta^{-2} + V_\infty,\ 4\pi^2\delta^{-2} + V_\infty\right]$$

The eigenvalues of the Intermediate Hamiltonian $L^D_{intm}$ coincide with the poles of the Intermediate DN-map $\mathcal{DN}_\Lambda$. Due to the the connection between the DN-map and the ND-map, $\mathcal{DN}_\Lambda\ \mathcal{ND}_\Lambda = I$, the eigenvalues of the Intermediate Hamiltonian therefore coincide with zeros of $\mathcal{ND}_\Lambda = I$.

Consider an isolated simple eigenvalue $\lambda^1_{intm}$ of the Intermediate Hamiltonian as a zero of $\mathcal{ND}_\Lambda = I$: $\mathcal{ND}_\Lambda(\lambda^1_{intm})e^1_{intm} = 0$, or $\mathcal{ND}_\Lambda(\lambda^1_{intm})Q^1_{intm} = 0$, with orthogonal projection $O_1 = e^1_{intm}\rangle\ \langle e^1_{intm}$. In terms of an orthogonal decomposition of $E_+ = E_1 \oplus E_1^\perp$ with $E_1 \equiv span\{e^1_{intm}\}$, the matrix of $\mathcal{ND}_\Lambda$ is represented as $\mathcal{ND}_\Lambda(\lambda) = d_1\,(\lambda - \lambda^1_{intm})\,Q^1_{intm} + \mathcal{ND}^\perp_\Lambda$ with $\mathcal{ND}^\perp_\Lambda(\lambda^1_{intm})$ invertible on $E_1^\perp$, or in matrix form

$$\mathcal{ND}^\perp_\Lambda(\lambda) = \begin{pmatrix} d_1(\lambda - \lambda^1_{intm}) & (\lambda - \lambda^1_{intm})\mathcal{ND}_{1\perp} \\ (\lambda - \lambda^1_{intm})\mathcal{ND}_{\perp 1} & \mathcal{ND}_{\perp\perp} \end{pmatrix}$$

analytic near $\lambda_1$ and with nontrivial residue $d_1 \neq 0$ and where $\mathcal{ND}_{\perp 1}(\lambda)$ can be calculated by the symmetry principle to be $\mathcal{ND} +_{1\perp} (\bar{\lambda})$. Then $\mathcal{DN}_\Lambda$ is also represented near $\lambda_1$ in the matrix form

$$\mathcal{DN}_\Lambda = \begin{pmatrix} d_1^{-1}(\lambda - \lambda^1_{intm})^{-1} & \mathcal{DN}_{1\perp} \\ \mathcal{ND} +_{1\perp} & \mathcal{DN}_{\perp\perp} \end{pmatrix} =: d_1^{-1}(\lambda^1_{intm})\frac{Q_1}{\lambda - \lambda^1_{intm}} + \mathcal{K}(\lambda), \quad (42)$$

with analytic bounded matrix elements $\mathcal{DN}_{1\perp}, \mathcal{DN}_{\perp\perp}$ uniquely defined near $\lambda_1$ by $d_1$ and the matrices $\mathcal{ND}_{1\perp}, \mathcal{ND}_{\perp\perp}$. Hence the scattering matrix near the zero $\lambda_1$ of the ND-map is represented as

$$S(\lambda) = \left[iK_+ + \frac{{d_1}^{-1}Q_1}{\lambda - \lambda^1_{intm}} + \mathcal{K}(\lambda)\right]^{-1} \left[iK_+ - \frac{{d_1}^{-1}Q_1}{\lambda - \lambda^1_{intm}} - \mathcal{K}(\lambda)\right]. \quad (43)$$

For thin junctions and low temperature the numerator and the denominator of the scattering matrix admit a rational approximation on the essential spectral interval $G_\Delta$ and it's complex neighborhood:

$$\begin{aligned} \mathcal{K}(\lambda) &= \mathcal{K}(\lambda^1_{intm}) + \left[\mathcal{K}(\lambda) - \mathcal{K}(\lambda^1_{intm})\right] \equiv \mathcal{K}(\lambda^1_{intm}) + \delta\mathcal{K}(\lambda),\ \lambda \in G_\Delta, \\ iK_+ - \frac{{d_1}^{-1}Q_1}{\lambda - \lambda^1_{intm}} - \mathcal{K}(\lambda) &\approx iK_+ - \frac{{d_1}^{-1}Q_1}{\lambda - \lambda^1_{intm}} - \mathcal{K}(\lambda^1_{intm}) \end{aligned}$$

if the error $\delta\mathcal{K}(\lambda)$ is dominated by $K_+$. Then the scattering matrix can be approximated, on an essential part of the neighborhood $G_\Delta$ (not too close to the zeros of the approximations:

$$S(\lambda) \approx S_{appr}(\lambda) = \left[iK_+ + \frac{{d_1}^{-1}Q_1}{\lambda - \lambda^1_{intm}} + \mathcal{K}(\lambda^1_{intm})\right]^{-1} \left[iK_+ - \frac{{d_1}^{-1}Q_1}{\lambda - \lambda^1_{intm}} - \mathcal{K}(\lambda^1_{intm})\right]. \quad (44)$$

In that case the resonances of the full scattering matrix can be calculated approximately using of the operator-valued Rouche theorem, see [45] and Appendix 3 below, based on the rational approximation (42) of $\mathcal{DN}_\Lambda$ on a complex neighborhood $G_\Delta$ of the essential spectral interval $\Delta_T$.

In the case when there are few eigenvalues of the Intermediate Hamiltonian $\lambda^s_{intm},\ s = 1, 2 \dots N_{\Delta_T}$ on the essential spectral interval $\Delta_T$, we can use the corresponding few-pole rational approximation of the intermediate DN-map

$$\mathcal{DN}_\Lambda = \sum_{\lambda^s_{intm} \in \Delta_T} (d_s)^{-1} \frac{Q_s}{\lambda - \lambda^1_{intm}} + \mathcal{K}(\lambda) = \sum_{\lambda^s_{intm} \in \Delta_T} (d_s)^{-1} \frac{Q_s}{\lambda - \lambda^1_{intm}} + \mathcal{K}_{\Delta_T}(\lambda) + \delta\mathcal{K}(\lambda) \quad (45)$$

with a rational hermitian matrix function $\mathcal{K}_{\Delta_T}$ regular on $G_\Delta$, and a small error $\delta\mathcal{K}(\lambda)$. Under the condition of domination for thin junction, that is $\parallel K_+^{-1}\delta\mathcal{K}(\lambda) \parallel < 1$ on the complex neighborhood $G_\Delta$, we can substitute the intermediate DN- map on $G_\Delta$ by the leading terms of the rational approximation

$$\mathcal{DN}_\Lambda \longrightarrow \sum_{\lambda^s_{intm} \in \Delta_T} (d_s)^{-1} \frac{Q_s}{\lambda - \lambda^s_{intm}} + \mathcal{K}_{\Delta_T}(\lambda) \equiv \mathcal{DN}_\Lambda^{\Delta_T},$$

so that the zeros of $iK_+ - \mathcal{DN}_\Lambda$ and the zeros of $iK_+ - \mathcal{DN}_\Lambda^{\Delta_T}$ do not deviate too much from each other, due to matrix Rouche theorem. Then on a major part of the complex neighborhood $G_\Delta$ of the essential spectral interval $\Delta_T$ - not too close to zeros of the numerator and the denominator of the "approximate" scattering matrix- we have

$$S \approx S_{appr} = \frac{iK_+ + \mathcal{DN}_\Lambda^{\Delta_T}}{iK_+ - \mathcal{DN}_\Lambda^{\Delta_T}}. \quad (46)$$

Unfortunately the matrix Rouche theorem gives only an estimation of the deviation of zeros of the perturbed matrix function from the zeros of the non-perturbed one, but does not provide a convergent process for calculation of the perturbed zeros. A construction of such an algorithm, especially in the case of several zeros of the unperturbed matrix function on $G_{\Delta_T}$, remains an important problem of analytic perturbation theory of Quantum Networks. We discuss this in the next section.

## 4. A Krein formula with compensated singularities for the intermediate DN-map

The semi-analytic approach to the calculation of the scattering matrix described in the previous section does not reveal the intuitively expected connection between the eigenvalues of the Dirichlet Schrödinger operator on the vertex domain of the junction and the resonances. On

the other hand, the standard technique of analytic perturbation theory, based on comparison of the resolvents $R^A_\lambda$, $R^{A_0}_\lambda$ of the unperturbed and the perturbed operators $A_0$, $A = A_0 + V$, yield the Lippmann-Schwinger equation, [62],

$$R^A_\lambda = R^{A_0}_\lambda - R^{A_0}_\lambda V R^A_\lambda,$$

with singularities on the spectrum of the unperturbed operator in both terms of the right side. This prevents straightforward use of the Lippmann-Schwinger equation for the calculation of scattered waves and the scattering matrix. Practical use of this equation in the 1D case shows however, that the singularities of the solution at the spectrum of the unperturbed operator are compensated.

In this section, following [29], we propose a modified analytic perturbation procedure to observe the compensation of singularities on the spectrum of the unperturbed operator in the solution of the Lippmann-Schwinger equation. The proposed semi-analytic construction allows us to avoid the singularities on the spectrum of the unperturbed operator and reveal the influence of the perturbation on the scattering matrix already on the first step of the perturbation procedure, under condition that the junction is "relatively thin".

We assume that the temperature $T$ is *low*, so that the essential spectral interval $\Delta_T$ lies within the conductivity band $\Delta_1 = [\lambda_{max}, \lambda_{min}]$ between the lower threshold $\lambda_{min}$ of the closed channels and the upper threshold $\lambda_{max}$ of the open channels.

In the case when the conductivity band is just the first spectral band we have $\Delta_1 = [\pi^2\,\delta^{-2} + V_\infty,\, 4\pi^2\,\delta^{-2} + V_\infty]$. Our prime aim here is to construct a rational approximation of the relative DN-map at (15) of the Intermediate Hamiltonian:

$$\mathcal{DN}_\Lambda g = \mathcal{DN}_{++} g - \mathcal{DN}_{+-} \frac{I}{\mathcal{DN}_{--} + K_-} \mathcal{DN}_{-+} g \tag{47}$$

on an essential part $\Delta_T$ of the first spectral band, taking into account the compensation of singularities on the spectrum of the unperturbed operator.

We represent the relative DN-map $\mathcal{DN}$ of $L^D_{int}$ on the essential spectral interval as a sum

$$\mathcal{DN} = \mathcal{DN}^{\Delta_T} + \mathcal{K} \tag{48}$$

of the rational expression constituted by the polar terms at the eigenvalues of the Dirichlet Schrödinger operator $L^D_{int}$, $\lambda_s \in \Delta_T$. We use this rational approximation on a complex neighborhood $G_{\Delta_T}$ of $\Delta_T$. We will use also matrix elements of $\mathcal{DN}$ obtained via framing it by the projections $P_\pm$, for instance

$$P_+ \mathcal{DN} P_- = P_+ \mathcal{DN}^{\Delta_T} P_- + P_+ \mathcal{K} P_- := \mathcal{DN}^{\Delta_T}_{+-} + \mathcal{K}_{+-}.$$

Due to the spectral representation of $\mathcal{DN}$, see [26], we have

$$\mathcal{DN}^{\Delta_T}_{+-} = \sum_{\lambda_s \in \Delta_T} \frac{P_+ \frac{\partial \varphi_s}{\partial n} \rangle\langle P_+ \frac{\partial \varphi_s}{\partial n}}{\lambda - \lambda_s}, \tag{49}$$

where $\varphi_s$ are the eigenfunctions of $L^D_{int}$ on $\Delta_T$.

We introduce also the linear hull $E^{\Delta_T} = \bigvee_s \{\varphi_s\}$ - an invariant subspace of $L^D_{int}$ corresponding to the essential spectral interval $\Delta_T$ and the part $L^{\Delta_T} := \sum_{\lambda_s \in \Delta_T} \lambda_s \varphi_s \rangle\langle \varphi_s$ of $L^D_{int}$ in the invariant subspace. To reveal the compensation of the singularities in $\mathcal{DN}_\Lambda$ arising from the spectrum of $L^D_{int}$, we need to solve the equation:

$$[\mathcal{DN}_{--} + K_-] u = \mathcal{DN}_{-+} g$$

on the essential spectral interval $\Delta_T$. We are able to do that based on an analytic perturbation procedure if $K_-$ can play the role of a large parameter on the essential spectral interval $\Delta_T$ so that the inverse $[\mathcal{K}_{--} + K_-]^{-1}$ exists on $\Delta_T$.

Denote by $\mathcal{T}$ the map

$$\mathcal{T} = \sum_{\lambda_s \in \Delta_T} \varphi_s \rangle \langle \frac{\partial \varphi_s}{\partial n}\Big|_{\Gamma} : E \longrightarrow E^{\Delta_T}$$

and introduce $Q(\lambda)$, $\mathcal{J}(\lambda)$ by

$$\mathcal{T}\frac{I}{\mathcal{K}_{--}+K_-}\mathcal{T}^+ \;:=\; Q(\lambda) : E_{\Delta_T} \longrightarrow E^{\Delta_T}, \to E_{\Delta_T} \tag{50}$$

$$\left(P_+ - \mathcal{K}_{+-}P_-\frac{I}{\mathcal{K}_{--}+K_-}P_-\right) \;:=\; \mathcal{J}(\lambda) :\; E \longrightarrow E_+ \tag{51}$$

A direct calculation, see [29], shows that the singularities in the first and second terms of (15) inherited from the non-perturbed operator are mutually compensated:

**Theorem 4.1. Compensation of singularities** *If $K_-$ can play the role of a large parameter on the essential spectral interval $\Delta_T$, then the intermediate DN-map can be represented on $\Delta_T$ as*

$$\mathcal{DN}_\Lambda = \mathcal{K}_{++} - -\mathcal{K}_{+-}\frac{I}{\mathcal{K}_{--}+K_-}\mathcal{K}_{-+} \; + P_+\mathcal{J}\mathcal{T}^+\rangle\frac{I}{\lambda I - L^{\Delta_T} + Q(\lambda)}\langle \mathcal{T}\mathcal{J}^+P_+. \tag{52}$$

*Proof* We begin with the standard Krein formula (47) for the DN-map of the intermediate operator $L^D_\Lambda$ on the essential spectral interval $\Delta_T$. Denote by $\mathcal{DN}^{\Delta_T}$ the component of the DN-map of $L_{int}$ on $\Delta_T$ defined by the formula (49), and introduce similar notations for the matrix elements of $\mathcal{DN}$ with respect to the orthogonal decomposition $E = E_+ \oplus E_-$, for instance

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

To calculate explicitly the second addendum in (47) we must solve the equation:

$$(\mathcal{DN}_{--} + K_-)\, u = \mathcal{DN}_{-+} g.$$

Using the local spectral representations of the above matrix elements of the rational approximation $\mathcal{DN}^{\Delta_T}$ on $\Delta_T$, we get:

$$\mathcal{DN}^{\Delta_T}_{--} = P_- \sum_{\lambda_s \in \Delta_T} \mathcal{T}^+\frac{I}{\lambda I^{\Delta_T} - L^{\Delta_T}}\mathcal{T}\; P_-,\;\; \mathcal{DN}^{\Delta_T}_{-+} = P_- \sum_{\lambda_s \in \Delta_T} \mathcal{T}^+\frac{I}{\lambda I^{\Delta_T} - L^{\Delta_T}}\mathcal{T}\; P_+.$$

Then, using the notation

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

and invertibility of $(K_- + \mathcal{K}_{--})$ we re-write the above equation

$$\left[\mathcal{DN}^{\Delta_T}_{--}u + (K_- + \mathcal{K}_{--})\right] u = \left[\mathcal{DN}^{\Delta_T}_{-+} + \mathcal{K}_{-+}\right] g$$

as

$$\frac{I}{K_- + \mathcal{K}_{--}}\; \mathcal{DN}^{\Delta_T}_{--}u + u = \frac{I}{K_- + \mathcal{K}_{--}}\left[\mathcal{DN}^{\Delta_T}_{-+} + \mathcal{K}_{-+}\right] g. \tag{53}$$

Using this notation $L^{\Delta_T}$, $\mathcal{T}, Q$ and the relevant representations for the matrix elements of the rational approximation of the standard DN-map, we obtain the following convenient equation for $V$

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

and the corresponding representation for $\mathbf{v}$

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

having in mind that the summation over $s$ is extended on the set of all eigenvalues of $L_{int}$ situated on the essential spectral interval $\Delta_T$. In this way we are able to calculate, based on (53),

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

Thus

$$\begin{aligned} \mathcal{DN}^F g &= \mathcal{DN}_{++}^{\Delta_T} g + \mathcal{K}_{++} g - \mathcal{DN}_{+-}^{\Delta_T} u - \mathcal{K}_{+-} u \qquad (54) \\ &= P_+ \mathcal{T}^+ \frac{I}{\lambda I^{\Delta} - L^{\Delta}} \mathcal{T} P_+ g + \mathcal{K}_{++} g - P_+ \mathcal{T}^+ \frac{I}{\lambda I^{\Delta} - L^{\Delta}} \mathcal{T} P_- u - \mathcal{K}_{+-} u \\ &:= I_1 + I_2 + I_3 + I_4, \end{aligned}$$

where the most complicated term is

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

We now insert these calculations into formula (54) and collect the terms in the right hand side which contain the second power of $[\lambda I^{\Delta} - L^{\Delta}]^{-1}$. Thus

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

Once this is done, we combine it with $I_1$ to see

$$\begin{aligned} P_+ T^+ \frac{I}{\lambda I^{\Delta} - L^{\Delta}} \mathcal{T} P^+ g - P_+ \mathcal{T}^+ \frac{I}{\lambda I^{\Delta} - L^{\Delta}} \frac{I}{\lambda I^{\Delta} - L^{\Delta} + Q} T P_+ g &= P_+ \mathcal{T}^+ \frac{I}{\lambda I^{\Delta} - L^{\Delta} + Q} \mathcal{T} P_+ g \\ &:= J_1 g. \end{aligned}$$

Next we combine the terms $I_{32}+I_{34}$ and $I_{31}+I_{33}$ containing $[\lambda I^\Delta - L^\Delta]^{-1}$:

$$\begin{aligned} I_{32}+I_{34} &= -P_+\mathcal{T}^+\frac{I}{\lambda I^\Delta - L^\Delta}\left[-I+Q\frac{I}{\lambda I^\Delta - L^\Delta+Q}\right]\mathcal{T}\frac{I}{K_-+\mathcal{K}_{--}}\mathcal{K}_{-+}g \\ &= -P_+\mathcal{T}^+\frac{I}{\lambda I^\Delta - L^\Delta+Q}\mathcal{T}\frac{I}{K_-+\mathcal{K}_{--}}\mathcal{K}_{-+}g \\ &:= J_2 g, \end{aligned}$$

and

$$\begin{aligned} I_{41}+I_{43} &= \mathcal{K}_{+-}\frac{I}{K_-+\mathcal{K}_{--}}\mathcal{T}^+\left[-I+\frac{I}{\lambda I^\Delta - L^\Delta+Q}Q\right]\mathcal{T}P_+g \\ &= -\mathcal{K}_{+-}\frac{I}{K_-+\mathcal{K}_{--}}\mathcal{T}^+\frac{I}{\lambda I^\Delta - L^\Delta+Q}\mathcal{T}P_+g \\ &:= J_3 g. \end{aligned}$$

We now see that no terms left in the right side of (54) with singularities $[\lambda I^\Delta - L^\Delta]^{-1}$ inherited from the unperturbed operator - all these singularities are compensated. Assembling separately the terms $J_1 g$, $J_2 g$, $J_3 g, I_{43}$ containing $[\lambda I^\Delta - L^\Delta + Q]^{-1}$ and the regular terms $I_2$, $I_{34}$ , we obtain the announced expression $\mathcal{DN}^F g$

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

The announced expression (52) for $\mathcal{DN}^F$ is now obtained from the above formula by introducing the notation

$$P_+ - \mathcal{K}_{+-}\frac{I}{K_-+\mathcal{K}_{--}} := \mathcal{J}$$

The derived formula is extended to a complex neighborhood $G_\Delta$ of the essential spectral interval using analyticity. Further analytical continuation is possible as well, but the estimates of leading and subordinate terms are obviously lost. □

The formula (52) contains details which should be calculated via an analytic perturbation procedure. If only a few steps are done in course of the calculation, we obtain an approximate expression $mathcalDN_\Lambda^{\Delta_T}$ for the intermediate DN-map with compensated singularities. For low temperature on a thin junction the approximate DN-map on $\Delta_T$ is just a finite sum of polar terms over the zeros $\lambda^s_{\Delta_T}$ of the denominator $\lambda I - L^{\Delta_T} + Q(\lambda)$ in (52) and a correction term $\mathcal{K}_\Delta(\lambda)$

which is regular on a complex neighborhood $G_{\Delta_T}$:

$$\mathcal{DN}_{\Lambda}^{\Delta_T} = \sum_{\lambda^s_{\Delta_T}\in\Delta} (d_s)^{-1}\frac{Q_s}{\lambda-\lambda^s_{\Delta_T}} + \mathcal{K}_{\Delta}(\lambda),$$

If the Fermi level $\Lambda$ is situated in the middle of the first spectral band, then for the thin junction the correcting term is dominated by the exponent $K_+$ in open channels and the scattering matrix can be estimated on a major part of $G_{\Delta_T}$ by the approximate expression

$$S_{appr} = \frac{iK_+ - \mathcal{DN}_{\Lambda}^{\Delta_T}}{iK_+ + \mathcal{DN}_{\Lambda}^{\Delta_T}}, \tag{55}$$

see an extended discussion of the one-pole approximation in [26].

## 5. A fitted zero-range solvable model for the quantum dot

The final expressions for the scattered waves on the junction in both preceding sections are obtained via matching of the standard scattering Ansatz in the wires $\omega$ with the solutions of the intermediate boundary problem on the vertex domain $\Omega_{int}$.

One can substitute the Intermediate Operator in this construction by a finite matrix which plays the role of the inner structure in the corresponding operator extension scheme, see [63]. The problem of constructing the zero-range solvable model of the junction is then reduced to fitting the inner structure and the boundary condition at the contact $\Gamma$ to the properties of the original problem for the Schrödinger operator in such a way that the model scattering matrix serves as an approximation of the original scattering matrix on a major part of the essential spectral interval $\Delta_T$, or on the major part of a complex neighborhood $G_{\Delta_T}$ of it.

Consider the Schrödinger operator $l_\Lambda$ on the open channels in $L_2(\omega)$

$$l_\Lambda U = -\frac{d^2U}{dx^2} + \sum_{s,m}\frac{\pi^2\, s^2}{\delta^2}\, p_s^m U + \mathbf{V}_\infty U,\ 0<x<\infty \tag{56}$$

defined on $W_2^2\left(E_+, \mathbb{R}_+\right)$, without boundary conditions at the origin. The boundary form of it is calculated via integration by parts:

$$\mathcal{J}_l(U,\, V) = \langle l_0^+ U,\, V\rangle - \langle U,\, l_0^+ V\rangle = \langle U'(0),\, V(0)\rangle - \langle U(0),\, V'(0)\rangle, \tag{57}$$

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

The construction of the vertex part of the model will be through a major change of the original Intermediate Hamiltonian. Without loss of generality we can assume that the essential spectral interval $\Delta_T$ lies strictly inside of the conductivity band - the first spectral band

$$\Delta_1 \subset [\lambda^{\Lambda}_{max},\, \lambda^{\Lambda}_{min}] = [\pi^2\delta^{-2} + V_{invty},\, 4\pi^2\delta^{-2} + V_{invty}]$$

and hence does not overlap with the continuous spectrum of the intermediate Hamiltonian $L_\Lambda$ , so that $\mathcal{DN}$ is selfadjoint on $\Delta_T$. As we have seen above, this assumption will be valid for thin junctions. According to [26] only a finite number $N$ of eigenvalues of the Intermediate Hamiltonian are situated on $\Delta_1 \supset \Delta_T$. We assume that there are some resonance eigenvalues situated on $\Delta_T$.

### 5.1. A solvable model of a quantum dot

The operator extension procedure was invented by J. von Neumann for densely defined symmetric operators. However, in our situation we see that the restriction of a finite matrix is not densely defined. Nevertheless, under a condition that the basic pair of the deficiency subspaces $N_i,\ N_{-i}$ are non-overlapping, a procedure of extension has been developed, see [51, 52, 63]. In this subsection we follow [63] in defining an operator extension procedure for the finite matrix.

Assume that the positive matrix $A$ has simple spectrum and is defined by the spectral decomposition

$$A = \sum_r \alpha_r^2\ P_r.$$

Here $\alpha_r^2 > 0$ are eigenvalues of $A$ and $P_r = \nu_r\rangle\,\langle\nu_r$ are the corresponding orthogonal spectral projections. The eigenvalues and the boundary parameters $\beta$ of the model, see below at (65), will be based on comparison of the scattering matrix of the model with the scattering matrix on $\Delta_T$.

Restriction of the matrix $A$ is equivalent to selection of the deficiency subspace for a given value of the spectral parameter. We choose the deficiency subspace $N_i$ as a generating subspace of

$$A : \overline{\bigvee_{k>0} A^k N_{-_i}} = E_A$$

such that

$$\frac{A+iI}{A-iI} N_i \cap N_i = 0, \quad \dim N_i = d$$

Set

$$D_0^A = (A - iI)^{-1}\,(E_A \ominus N_i)$$

and define the restriction of the inner Hamiltonian as $A \to A_0 = A\big|_{D_0^A}$. We develop the extension procedure for general $N_i$ and fit it later based on the spectral data of the intermediate operator, see Theorems 5.2 and 5.3. In our construction $N_i \subset E_A$ plays the role of the deficiency subspace at the spectral point $i$, dim $N_i = d,\ 2d \leqslant N$ 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 $E_A$, 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 [63]. In this case the "formal adjoint" operator for $A_0$ is defined on the defect $N_i + N_{-i} := \mathcal{N}$ by the von Neumann formula: $A_0^+ e \pm i\, e = 0$ for $e \in N_{\pm i}$. Then the extension is constructed 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 $V : N_i \to N_i$ in the form

$$\mathcal{T}_V = (I - V)\, N_i.$$

In the case when the deficiency subspaces do not overlap, the corresponding isometry is "admissible" and, according to [50], there exist a self-adjoint extension $A_V$ of the restricted operator $A_0$. We need the following

**Lemma 5.1.** *The Lagrangian plane $\mathcal{T}_V$ 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 $\mathcal{T}_V$ it coincides with the restriction of the formal adjoint, and on the domain $D_0^A$ it coincides with $A_0$. Then assuming that $\mathcal{T}_V$ 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 $f^{\perp}=-2i\nu=0$. □

It follows from the Lemma that, once the extension is constructed on the Lagrangian plane, the whole construction of the extended operator can be finalized as 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 the non-overlapping condition also, see [50]. In particular, in the case $\dim E_A=1$, which is not formally covered by the above procedure, was analyzed in [53] independently of [50]. The relevant formulas for the scattering matrix and scattered waves remain true and may be verified by the direct calculation. We will use this fact below.

Choose an orthonormal basis in $N_i$, say $\{f_s\}$, $s=1,2,\ldots,d$ a set of deficiency vectors of the restricted operator $A_0$. Then the vectors $\hat{f}_s=\frac{A+iI}{A-iI}f_s$ form an orthonormal basis in the dual deficiency subspace $N_{-i}$. Under the non-overlapping condition one can use the formal adjoint operator $A_0^+$ defined on the defect $N_i+N_{-i}=\mathcal{N}$:

$$u=\sum_{s=1}^{d}[x_s\,f_s+\hat{x}_s\,\hat{f}_s]\ \in\mathcal{N}, \tag{58}$$

by the von Neumann formula, see [18],

$$A_0^+u=\sum_{s=1}^{d}[-i\ x_s\,f_s+i\ \hat{x}_s\,\hat{f}_s]. \tag{59}$$

In order to use the symplectic version of the operator-extension techniques we need to introduce in the defect a new basis $w_{s,\pm}$, on which the formal adjoint $A_0^+$ is correctly defined due to the above non-overlapping condition:

$$\begin{aligned} w_{s,+} &= \frac{f_s+\hat{f}_s}{2}=\frac{A}{A-iI}f_s \\ w_{s,-} &= \frac{f_s-\hat{f}_s}{2i}=-\frac{I}{A-iI}f_s \end{aligned}$$

and so

$$A_0^+w_{s,+}=w_{s,-}\qquad A_0^+w_{s,-}=-w_{s,+}$$

It is convenient to represent elements $u\in\mathcal{N}$ via this new basis as

$$u=\sum_{s=1}^{d}[\xi_s^+\,w_{s,+}+\xi_s^-\,w_{s,-}]. \tag{60}$$

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

$$u=\frac{A}{A-iI}\vec{\xi}_+^{\,u}-\frac{1}{A-iI}\vec{\xi}_-^{\,u},\quad A_0^+u=-\frac{1}{A-iI}\vec{\xi}_+^{\,u}-\frac{A}{A-iI}\vec{\xi}_-^{\,u} \tag{61}$$

The following formula for "integration by parts" for abstract operators was proved in [63].

**Lemma 5.2.** *Consider the elements $u, v$ from the domain of the (formal) adjoint operator $A_0^+$:*

$$u = \frac{A}{A - iI}\vec{\xi}_+^u - \frac{1}{A - iI}\vec{\xi}_-^u,\ v = \frac{A}{A - iI}\vec{\xi}_+^v - \frac{1}{A - iI}\vec{\xi}_-^v$$

*with coordinates $\vec{\xi}_\pm^u$, $\vec{\xi}_\pm^v$:*

$$\vec{\xi}_\pm^u = \sum_{s=1}^{d} \xi_{s,\pm}^u f_{s,i} \in N_i,\ \vec{\xi}_\pm^v = \sum_{s=1}^{d} \xi_{s,\pm}^v f_s \in N_i.$$

*Then, the boundary form of the formal adjoint operator is equal to*

$$\mathcal{J}_A(u, v) = \langle A_0^+ u, v\rangle - \langle u, A_0^+ v\rangle = \langle \vec{\xi}_+^u, \vec{\xi}_-^v\rangle_N - \langle \vec{\xi}_-^u, \vec{\xi}_+^v\rangle_N. \tag{62}$$

One can see that the coordinates $\vec{\xi}_\pm^u$, $\vec{\xi}_\pm^v$ of the elements $u, v$ play the role of the boundary values similar to $\{U'(0),\ U(0),\ V'(0),\ V(0)\}$. We will call them *symplectic coordinates* of the element $u, v$. The next statement proved in [63] is the central feature of the fundamental Krein formula [18], for generalized resolvents of symmetric operators. In our situation, it is used in the course of the calculation of the scattering matrix.

**Lemma 5.3.** *The vector-valued function of the spectral parameter*

$$u(\lambda) = \frac{A + iI}{A - \lambda I}\ \vec{\xi}_+^u := u_0 + \frac{A}{A - iI}\vec{\xi}_+^u - \frac{1}{A - iI}\vec{\xi}_-^u, \tag{63}$$

*satisfies the adjoint equation $[A_0^+ - \lambda I]u = 0$, and the symplectic coordinates $\vec{\xi}_\pm^u \in N_i$ of it are connected by the formula*

$$\vec{\xi}_-^u = -P_{N_i}\frac{I + \lambda A}{A - \lambda}\vec{\xi}_+^u \tag{64}$$

We introduce the operator

$$P_{N_i}\frac{I + \lambda A}{A - \lambda I}P_{N_i} := \mathcal{M} : N_i \to N_i$$

It has a positive imaginary part in the upper half-plane $\Im m\ \lambda > 0$ and will serve us an abstract analog of the celebrated Weyl-Titchmarsh function, see [18, 42].

The operator $\mathcal{M}$ exists almost everywhere on the real axis $\lambda$ with a finite number of simple poles at the eigenvalues $\alpha_r^2$ of $A$. This function plays an important role in description of spectral properties of self-adjoint extensions of symmetric operators, see [64].

We construct a solvable model of the quantum network as a self-adjoint extension of the orthogonal sum $l_0 \oplus A_0$.

We begin with the orthogonal sum of the corresponding adjoint $l_0^+$ and the formal adjoint: $l_0^+ \oplus A_0^+$, and calculate the corresponding boundary form $\mathbf{J}(\mathbf{U}, \mathbf{V}) := \mathcal{J}(U, V) + \mathcal{J}(u, v)$ on elements $(U, u) := \mathbf{U}$ from the orthogonal sum of the corresponding spaces. The self-adjoint extensions of the operator $l_0 \oplus A_0$ are obtained, based on restrictions of the adjoint operator $\mathbf{A}_0^+ = l_0^+ \oplus A_0^+$ onto Lagrangian planes of the form $\mathbf{J}(\mathbf{U}, \mathbf{V})$. These planes may be defined by the boundary conditions connecting symplectic coordinates $U'(0),\ U(0),\ \vec{\xi}_+^u,\ \vec{\xi}_-^u$ of components of elements from the defect. For instance, one may select a finite-dimensional operator $\beta : E_+ \oplus N_i \to E_+ \oplus N_i$ and define the Lagrangian plane $\mathbf{L}_\beta$ by the boundary condition

$$\begin{pmatrix} U'(0) \\ -\vec{\xi}_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta_{10} & 0 \end{pmatrix} \begin{pmatrix} U(0) \\ -\vec{\xi}_- \end{pmatrix}. \tag{65}$$

The extension defined by (65) on the Lagrangian plane is continued onto the whole space $L_2(E_+,\ R_+) \oplus E_A$ by forming the direct sum with the closure of the restricted operator $A_0$,

see [50]. This construction gives a self-adjoint extension $\mathbf{A}_\beta$ of $l_0 \oplus A_0$ in $L_2(E_+, R_+) \oplus E_A$, defined by the boundary condition (65). The absolutely continuous spectrum of the operator $\mathbf{A}_\beta$ 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 $\mathcal{L}_\Lambda$ (in the open channels). The corresponding eigenfunctions of $\mathbf{A}_\beta$ on the maximal essential spectral band $\left[\lambda^\Lambda_{\max},\ \lambda^\Lambda_{min}\right] \supset \Lambda$ can be found, via substitution into the above boundary condition the column formed from of the scattering Ansatz in open channels with (63) and in the outer space:

$$\vec{\Psi} = \begin{pmatrix} e^{iK_+x}\nu + e^{-i\,K_+x}\mathbf{S}\nu \\ \frac{A+iI}{A-\lambda I}\vec{\xi}^u_+ \end{pmatrix}. \tag{66}$$

In this way we obtain a linear equation for the scattering matrix:

$$\begin{pmatrix} iK_+\,(\nu - S\nu) \\ -\vec{\xi}_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta_{10} & 0 \end{pmatrix} \begin{pmatrix} \nu + \mathbf{S}\nu \\ \mathcal{M}\vec{\xi}_+ \end{pmatrix}.$$

Upon solving this equation we obtain the scattered waves and the scattering matrix:

**Theorem 5.1.** *The scattering matrix for the constructed extension is an analytic function of the spectral parameter $\lambda$:*

$$\mathbf{S}(\lambda) = \frac{iK_+ - [\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}]}{iK_+ + [\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}]}, \tag{67}$$

Of course we mean here

$$\mathbf{S}(\lambda) = \big(iK_+ - [\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}]\,\big)\big(iK_+ + [\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}]\,\big)^{-1} \tag{68}$$

*Proof.* We eliminate $\vec{\xi}_+$ from the preceding equation. The vector $\nu$ is a free parameter, and the coordinate $\vec{\xi}_+$ of the inner component of the scattered wave (66) is defined as $\vec{\xi}_+ = -\beta_{10}(I + \mathbf{S})\nu$. □

### 5.2. Fitting the solvable model

The comparison of the ultimate expression (67) for the scattering matrix of the model junction with the approximate expressions (46) and (55) reveals a similar structure between all of these expressions and thus creates hope that the parameters $A, N_{\pm i}, \beta$ of the extension can be selected so that the model scattering matrix coincides with one of the approximate scattering matrices.

Consider the approximate scattering matrix (46) with

$$\mathcal{DN}^{\Delta_T}_\Lambda = \sum_{r=1}^{N} \frac{P_+\frac{\partial\varphi^\Lambda_r}{\partial n}\rangle\langle P_+\frac{\partial\varphi^\Lambda_r}{\partial n}}{\lambda - \lambda^\Lambda_r} + \mathcal{K}^{\Delta_T}(\lambda) \tag{69}$$

with polar terms constituted by the projections onto the boundary currents of the eigenfunctions $\varphi^\Lambda_r$ of the Intermediate Hamiltonian which correspond to the eigenvalues $\lambda^\Lambda_r$ on the essential spectral interval $\Delta_T$, and a regular on $G_{\Delta_T}$ correcting term $\mathcal{K}^{\Delta_T}(\lambda)$.

It remains to choose the parameters $A, N_{\pm i}, \beta$ of the model such that the operator-function $[\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}]$ acting in $E_+$ coincides with the essential DN-map $\mathcal{DN}^\Delta_\Lambda$ of the Intermediate Hamiltonian on $\Delta_T$. Denote by $Q_s$ the spectral projection $P^A_s = \nu_{\alpha_s}\rangle\,\langle\nu_{\alpha_s}$ of the operator $A$ corresponding to the simple eigenvalue $\alpha^2_s$ , framed by the projections $P_i$ onto the deficiency subspace $N_i$

$$Q_s = P_i P_s P_i.$$

Then the expression $[\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}]$ takes the form:

$$[\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}] = \left[\beta_{00} + \sum_{r=1}^{N_T} \alpha_r^2 \beta_{01} Q_s \beta_{10}\right] + \sum_r \frac{1+\alpha_r^4}{\lambda - \alpha_r^2}\beta_{01} Q_r \beta_{10}. \tag{70}$$

We will define the boundary parameters $\beta_{10}$, $\beta_{01} = \beta_{10}^+$ later, but once they are defined, we choose $\beta_{00}$ such that the first summand in the right side of (70) vanishes:

$$\beta_{00} = -\sum_r \alpha_r^2 \beta_{01} Q_r \beta_{10} \tag{71}$$

Then the scattering matrix takes a form similar to (69). Note that for the junctions under consideration the leading term $iK+$ dominates the regular error, both in (67) and in (46). In order to to fit the model we should choose the eigenvalues of $A$ equal to the eigenvalues of the intermediate hamiltonian on the essential spectral interval $\Delta_T$.

Summarizing these results we obtain the following conditional statement for the extension constructed based on the boundary condition (65) in case when $N_i \cap N_{-i} = 0$ or dim $E_A = 1$:

**Theorem 5.2.** *The constructed operator $\mathbf{A}_\beta$ is a solvable model of the Quantum network on the essential spectral interval $\Delta_T$, if and only if the dimension of the space $E_A$ coincides with the number $N$ of eigenvalues of the intermediate operator on $\Delta_T \subset [\lambda_{max}, \lambda_{min}] = \Delta_1$, the eigenvalues $\alpha_r^2$ of the inner Hamiltonian $A = \sum_{r=1}^N \alpha_r^2 \nu_{\alpha_r}\rangle\langle\nu_{\alpha_r}$ coincide with the eigenvalues of the Intermediate Hamiltonian on $\Delta_T$, there exists a deficiency subspace $N_i$ of the inner Hamiltonian such that $N_i \cap \frac{A+iI}{A-iI}N_i = 0$ and the operator $\beta_{01} : N_i \to E_+$ such that for the ortho-normal basis $\{e_s\}_{s=1}^N$ of eigenvectors of $A$ in $E_A$*

$$P_+ \frac{\partial \phi_r}{\partial n} = [1 + \alpha_r^4]^{1/2} \beta_{01} P_i \nu_{\alpha_r},\ r = 1, 2, \ldots, N. \tag{72}$$

Harmer has suggested an important strengthening of the previous conditional statement, by proving a general theorem concerning the existence of the subspace $N_i$ and the projection $P_{Ni}$ which satisfying the conditions of Theorem 5.2

Denote by $L_\Lambda^\Delta$ 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

$$\sum_s [1 + \alpha_s^4]^{-1/2} P_+ \frac{\partial \varphi_s}{\partial n}\bigg|_\Gamma \langle *, \varphi_s\rangle := \Phi_\Delta \tag{73}$$

from $E_\Delta$ to $E_+$, and set dim($E_+$) =**n** .

**Theorem 5.3.** *(Harmer) The map $\Phi_\Delta$ defines a one-to one correspondence between the two $d$-dimensional subspaces, $2d < N$:*

$$\Phi_\Delta^+ \Phi_\Delta E_\Delta := N_\Delta \subset E_\Delta \ \text{ and } \ \Phi_\Delta \Phi_\Delta^+ E_+ := E_+^\Delta \subset E_+$$

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

$$N_\Delta \cap \left(L_\Lambda^\Delta - iI\right)^{-1}\left(L_\Lambda^\Delta + iI\right) N_\Delta = 0, \tag{74}$$

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

The proof for this statement can be found in [54]

In the case when there is only one resonance eigenvalue $\alpha_0^2$ of the Intermediate Hamiltonian sits on $\Delta_T$, we obtain the model scattering matrix

$$\mathbf{S}(p) = \frac{K_+ - \frac{1+\alpha_0^4}{\alpha_0^2-\lambda}\beta_{01}Q_0\beta_{10}}{K_+ + \frac{1+\alpha_0^4}{\alpha_0^2-\lambda}\beta_{01}Q_0\beta_{10}} \tag{75}$$

which is a single-pole approximation of the scattering matrix of the thin 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 $E_+$ spanned by $P_+\frac{\partial\varphi_0}{\partial n}$. For thin or shrinking networks one can estimate, (see [26]), the deviation of the single-pole and/or few-poles approximations from the exact scattering matrix on the network, in terms of the ratio $d/\operatorname{diam}\Omega_{int}$. The local wave operators and the corresponding scattering matrix on the essential spectral band can be defined for the pair $(\mathcal{L}, \mathbf{A}_\beta)$, see [48].

## 6. Example: a zero-range solvable model as a kick-start in the analytic perturbation procedure

Consider a thin quantum network constructed of a model quantum well and a single thin quantum wire. 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 operator with $\hbar^2(2m^*)^{-1} = I$, $V + \pi^2\ \delta^{-2}\Big|_\omega = 0$, $K_+ = pI_+ = \sqrt{\lambda}\, I_+$ and the corresponding one-dimensional subspace $E_+$:

$$-u'' = p^2u,\ 0 < x < \infty. \tag{76}$$

This equation can be interpreted as a result of separating variables in the one-dimensional acoustic equation $u_{tt} - u_{xx} = 0$ on a semi-infinite string $R_+$. We connect the string with a resonator attached to the end $x = 0$, manufactured as a zero-range potential with an inner structure, see previous section. The corresponding quantum problem is reduces to the same stationary spectral problem with a threshold shifted from zero to the lower threshold $\pi^2\,\delta^{-2} + V_{infty}$ in the wire. In this section we assume that $\pi^2\,\delta^{-2} + V_{infty}$, keeping in mind that the shift of the threshold does not affect the analytic properties of the spectral problem. But the corresponding acoustic dynamical problem, second order in time, is substituted by the Schrödinger dynamic problem, first order in time. After an appropriate scaling of the time variable the quantum dynamic problem is reduced to the equation

$$\frac{1}{i}\,\frac{\partial\psi}{\partial t} + \frac{\partial^2\psi}{\partial x^2} = 0, \tag{77}$$

or a corresponding equation with a threshold shifted by an addition of a constant potential $V$ in thewires. Having in mind this connection, we continue analysis of the stationary spectral problem of the acoustic equation equipped by a zero-range potential, with inner structure, attached at the origin.

Assume that the model Hamiltonian $\mathbf{A}_\beta$ is constructed as suggested in the previous section based on the "inner Hamiltonian"$A = \sum_{s=1}^N \alpha_s^2\ \nu_s\rangle\,\langle\nu_s$, with selected 1D deficiency subspaces $N_{\pm i}$, corresponding projections $P_{\pm i} = e\rangle\,\langle e$, and the differential operator $l_\Lambda$ in the wire, linked to the inner structure via the hermitian matrix $\beta$ of the boundary parameters $\beta_{ik}$ selected as per

below:

$$\begin{pmatrix} iK_+\,(\nu - \mathbf{S}\nu) \\ -\vec{\xi}_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta_{10} & \beta_{11} \end{pmatrix} \begin{pmatrix} \nu + \mathbf{S}\nu \\ \mathcal{M}\vec{\xi}_+ \end{pmatrix},$$

with the Weyl function $\mathcal{M} = \mathrm{Trace} P_i \frac{I-\lambda A}{A-\lambda I}$. Hereafter we assume that the deficiency subspace $N_i = span\{\nu\}$ is identical to the cross-section subspace of the open channel $E_+ = span\ e = span\ \nu$. Then

$$P_i \frac{I-\lambda A}{A-\lambda I} P_i = \mathcal{M} P_i$$

Solving this equation gives us the scattered waves $e^{ipx} + e^{-ipx}\mathbf{S}$ and the scattering matrix $\mathbf{S}_\beta = S_\beta(\lambda)\ P_+$ which is defined for the constructed extension in the 1D cross-section subspace $E_+$ by the scalar function $\mathcal{M}$

$$S_\beta(\lambda) = \frac{ip - \left[\beta_{00} - \beta_{01}\frac{\mathcal{M}}{I+\beta_{11}\mathcal{M}}\beta_{10}\right]}{ip + \left[\beta_{00} - \beta_{01}\frac{\mathcal{M}}{I+\beta_{11}\mathcal{M}}\beta_{10}\right]}. \tag{78}$$

Hereafter we assume that the boundary parameter is connected with the inner structure and the deficiency subspaces by the condition $\beta_{11}\ \mathrm{Trace} P_i\ A = 1$. Then

$$\mathrm{Trace}\frac{I+\lambda A}{A-\lambda\, I} = -\mathrm{Trace} P_i\ A + \mathrm{Trace}\frac{I+A^2}{A-\lambda I},$$

and hence

$$1 + \beta_{11}\mathcal{M} = \beta_{11}\ \mathrm{Trace}\frac{I+A^2}{A-\lambda I}\ \ \frac{\mathcal{M}}{1+\beta_{11}\mathcal{M}} = \frac{-\mathrm{Trace} P_i\ A}{\beta_{11}\ \mathrm{Trace}\frac{I+A^2}{A-\lambda I}} + \frac{1}{\beta_{11}}$$

This gives us the scalar factor scattering matrix

$$S_\beta(\lambda) = \frac{ip - \beta_{00} + \beta_{01}\,\beta_{11}^{-}\,\beta_{10} + \beta_{01}\,\beta_{11}^{-2}\left[\mathrm{Trace}\ \frac{1+A^2}{\lambda I - A}P_i\right]^{-1}\ \beta_{10}}{ip + \beta_{00} - \beta_{01}\,\beta_{11}^{-2}\,\beta_{10} - \beta_{01}\,\beta_{11}^{-2}\left[\mathrm{Trace}\ \frac{1+A^2}{\lambda I - A}P_i\right]^{-1}\ \beta_{10}}, \tag{79}$$

which tends to $-1$ at infinity in the complex plane, $\lambda = p^2 \to \infty$, similarly to the scattering matrix of the Dirichlet Schrödinger operator on a half-axis. On the other hand, the scattering matrix reveals a peculiar behavior near the eigenvalues of the inner structure when the interaction between the inner structure and the outer space is switched off. Indeed, let us assume that $\lambda = p^2$ is near to $\alpha_r^2$, or $p \approx \pm\alpha_r$. Then the leading term of

$$\left[\mathrm{Trace}\ \frac{1+A^2}{\lambda I - A}P_i\right] = \frac{1+\alpha_r^4}{\lambda - \alpha_r^2}\parallel P_i\nu_r \parallel^2 + \sum_{s\neq r}\frac{1+\alpha_s^4}{\lambda-\alpha_s^2}\parallel P_i\nu_s\parallel^2 \equiv \frac{1+\alpha_r^4}{\lambda-\alpha_r^2}\parallel P_i\nu_r\parallel^2 + \gamma_r(\lambda)$$

is represented at $\lambda \approx \alpha_r^2$ by the polar expression which dominates the bounded correcting term $\gamma_r(\lambda)$. Then the scattering matrix near $\alpha_r^2$ is calculated as

$$S_\beta(\lambda) = \frac{ip - \det\beta\ \beta_{11}^{-1} + \frac{|\beta_{01}|^2}{\beta_{11}^2}(1+\alpha_r^4)\left[\frac{\lambda-\alpha_r^2}{1+\frac{\lambda-\alpha_r^2}{1+\alpha_r^4}\gamma_r(\lambda)}\right]\parallel P_i\nu\parallel^{-2}}{ip + \det\beta\ \beta_{11}^{-1} - \frac{|\beta_{01}|^2}{\beta_{11}^2}(1+\alpha_r^4)\left[\frac{\lambda-\alpha_r^2}{1+\frac{\lambda-\alpha_r^2}{1+\alpha_r^4}\gamma_r(\lambda)}\right]\parallel P_i\nu\parallel^{-2}} \approx$$

$$S_\beta(\lambda) = \frac{ip - \det\beta\ \beta_{11}^{-1} + \frac{|\beta_{01}|^2}{\beta_{11}^2}(1+\alpha_r^4)(p^2-\alpha_r^2)\parallel P_i\nu\parallel^{-2}}{ip + \det\beta\ \beta_{11}^{-1} - \frac{|\beta_{01}|^2}{\beta_{11}^2}(1+\alpha_r^4)(p^2-\alpha_r^2)\parallel P_i\nu\parallel^{-2}}. \tag{80}$$

This formula becomes exact if the inner structure is one-dimensional, $r = 1, \gamma_r = 0$. This fact will be used in next section. But it may also serve a convenient approximation for the scattering matrix anyway in the case when $|\beta_{01}|^{-2} \to 0,\ \det\beta\ |\beta_{01}|^{-2} \to 0$. In particular, the poles of the scattering matrix - the resonances - are calculated under this condition , for small $|\beta_{01}|^{-2}, \det\beta\ |\beta_{01}|^{-2}$ as

$$p_r(\beta) \approx \alpha_r + \frac{1+\alpha_r^4}{2}\left[i\frac{\beta_{11}^2}{|\beta_{01}|^2} + \frac{\beta_{11}\ \det\beta}{\alpha_r|\beta_{01}|^2}\right].$$

In particular, for $\det\beta = 0$, the displacement of the resonance $p_r(\beta)$ from the limiting position at large $\beta$ in $\alpha_r$ is just vertical and does not require any conditions, except the switching off the interaction $\beta_{01} \to \infty$ between the wire and the vertex domain of the junction.

Summarizing our results, we obtain the following statement:

**Theorem 6.1.** *The scattering matrix (79) is unitary on the real axis of the $p$-plane and has zeros at the points $\bar{p}_s(\beta)$ in the lower half-plane, and poles in the complex conjugate points $p_s(\beta)$ in the upper half-plane $\Im m(p) > 0$, situated symmetrically with respect to the imaginary axis of this $p$-plane. It is an analytic function of the spectral parameter $\lambda$, but it is not analytic with respect to the coupling parameter $\det\beta$, $|\beta_{01}|^{-2} \to 0$. In particular, if the inner structure $A$ is fixed, $A = \sum_s \alpha_s^2 \nu_s\rangle\langle\nu_s$, and the coupling parameter is selected such that*

$$\beta_{11} TraceAP_i = 1,\ |\beta_{01}|^{-2} \to 0 \textit{ and, simultaneously } \det\beta\,|\beta_{01}|^{-2} \to 0, \tag{81}$$

*then the inner and the outer components of the junction are decoupled, in the limit (81), and the poles $p_s(\beta)$ depend on $\beta^{-1}, \to 0$, $\det\beta\,|\beta_{01}|^{-2} \to 0$ analytically and approach the real points $\pm\alpha_r = \pm\sqrt{\alpha_s^2}$ as*

$$p_s(\beta) = \alpha_s + i\frac{\beta_{11}(1+\alpha_r^4)}{2|\beta_{01}|^2} + \frac{(1+\alpha_r^4)\det\beta}{2\,\alpha_r\,|\beta_{01}|^2} + \dots \tag{82}$$

Even in the case of 1D inner structure the factor (80) of the scattering matrix is not analytic with respect to $\beta^{-1}, \det\beta\,|\beta_{01}|^{-2}$ , because the zeros $p_r$ of both the numerator and the denominator approach the same points $\pm\alpha_r$ when $\beta^{-1}, \to 0$, $\det\beta\,|\beta_{01}|^{-2} \to 0$, hence the scattering matrix (79) nor the scattered wave depend analytically on the boundary parameter $\beta^{-1}$ on the product of a small neighborhood of the origin in $\beta^{-1}$ - space and small neighborhoods of $p_s(0)$ in $p$-plane. The analyticity is actually lost due to *creation of resonances* at the points $p_s 0 = \pm\alpha_s$, when the interaction between the inner and the outer components of the junction, initially decoupled ,$\beta^{-1} = 0$, is *switched on*, when the boundary parameter $\beta^{-1}$ exits from the origin.

### 6.1. Acoustic analog of a quantum dot and the chain rule for the scattering matrices

Both the Schrödinger equation and the acoustic equation are reduced to the spectral problem for the second order selfadjoint diffential operator. The only technical detail distinguishing the spectral problems is the threshold of the continuous spectrum , which is zero in the case of the acoustic problem defining the absence of the waves diffusion and existence of the functional-invariant solutions represented in 1D case by Dalambertian waves $\Psi(x \pm t)$. In this section we consider the scattering problem for acoustic junction based on the equation second order in time:

$$\frac{\partial^2}{\partial t^2}\begin{pmatrix}\Psi\\ \psi\end{pmatrix} + \mathbf{A}_\beta\begin{pmatrix}\Psi\\ \psi\end{pmatrix} = 0.$$

on a half-axis with the boundary condition at the end $x = 0$ defined by the inner Hamiltonian $A$ and the boundary condition

$$\begin{pmatrix} \frac{\partial\Psi(x)}{\partial x}\Big|_0 \\ -\vec{\xi}_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta_{10} & \beta \end{pmatrix} \begin{pmatrix} \Psi(x)\Big|_0 \\ -\vec{\xi}_- \end{pmatrix}, \tag{83}$$

imposed onto the boundary data $\frac{\partial\Psi}{\partial x}\Big|_{x=0}$, $\Psi\Big|_{x=0}$ of the outer component of the solution and the boundary data $\xi_+, \xi_-$ of the inner component $\psi$ of the solution $\vec{\Psi} = (\Psi, \psi)$ of the wave equation $\vec{\mathbf{\Psi}}_{tt} + \mathbf{A}_\beta\vec{\mathbf{\Psi}} = 0$ at the contact of the inner and the outer components of the junction. In terms of Cauchy data $(\vec{\Psi}, \frac{\partial\vec{\Psi}}{\partial t}) \equiv \vec{\mathbf{\Psi}}$ the acoustic equation can be represented , see [30] , as

$$\frac{1}{i}\frac{\partial}{\partial t}\vec{\mathbf{\Psi}} = i\begin{pmatrix} 0 & -1 \\ \mathbf{A}_\beta & 0 \end{pmatrix}\vec{\mathbf{\Psi}} \equiv \mathcal{L}_\beta\ \vec{\mathbf{\Psi}}. \tag{84}$$

The spectrum of the Lax-Phillips generator $\mathcal{L}_\beta$ is purely continuous multiplicity 1 on $(-\infty, \infty)$, and the eigenfunctions of thew continuous spectrum are the scattered waves constructed as columns

$$\vec{\mathbf{\Psi}} = \begin{pmatrix} \frac{1}{ip} \\ 1 \end{pmatrix}\vec{\Psi},$$

with $\vec{\Psi}$ defined by (66) with $K_+ = p$ in this subsection. The generator $\mathcal{L}_\beta$ of the Lax-Phillips evolution group defined by the wave equation 84 is unitary with respect to the energy norm defined on the Cauchy data $\vec{\mathbf{\Psi}} \equiv \left(\vec{\Psi}, \frac{\partial\vec{\Psi}}{\partial t}\right))$ as

$$\parallel \vec{\mathbf{\Psi}} \parallel^2_{\mathcal{E}} = \frac{1}{2}\int_0^\infty \left[\left|\frac{\partial Psi}{\partial x}\right|^2 + \left|\frac{\partial\Psi}{\partial t}\right|^2\right] dx + \frac{1}{2}\left[\langle A\psi,\, \psi\rangle + \parallel \psi_t \parallel^2\right] + \frac{1}{2}\langle\beta\begin{pmatrix} \Psi(0) \\ -\xi^\psi_- \end{pmatrix}, \begin{pmatrix} \Psi(0) \\ -\xi^\psi_- \end{pmatrix}\rangle, \tag{85}$$

and the evolution group is unitary in the energy-normed space $\mathcal{E}$ of the Cauchy data of the acoustic problem. The spectral representation of the group is represented in terms of the scattered waves $\vec{\mathbf{\Psi}}_p$

$$\vec{\mathbf{\Psi}}(x,t) = \frac{1}{2\pi}\int_R \vec{\mathbf{\Psi}}_p(x)\rangle\ e^{ipt}\langle\vec{\mathbf{\Psi}}_p, \vec{\mathbf{\Psi}}(*,0)\rangle_{\mathcal{E}}dp$$

which transfers the Cauchy data of the incoming waves in the wire $\Psi(x+t)$ into the Hardy class $H^2_-$ of all square-integrable functions which admit an analytic continuation into the lower half-plane, and the Cauchy data of the outgoing waves $\Psi(x-t)$ on the wire into the invariant subspace $S^+H^2_+$ of the hardy class $H^2_+$ in the upper half-plane. The corresponding spectral duality is established by the formulae

$$\vec{\mathbf{U}} \equiv \begin{pmatrix} U \\ u \end{pmatrix} \xrightarrow{J_\mathcal{E}} \frac{1}{\sqrt{2\pi}}\langle\vec{\mathbf{\Psi}}_p, \vec{\mathbf{U}}\rangle_\mathcal{E} \equiv J_\mathcal{E}\vec{\mathbf{U}}$$

$$J_\mathcal{E}\vec{\mathbf{U}} \xrightarrow{J^+_\mathcal{E}} \frac{1}{\sqrt{2\pi}}\int_R \mathbf{\Psi}_p\ J_\mathcal{E}\vec{\mathbf{U}}dp = \vec{\mathbf{U}}, \tag{86}$$

and the inner space $E_A \oplus E_A \equiv K$ of the system is transferred by $J_\mathcal{E}$ into $H^2_+ \ominus \mathbf{S}_{LPh}\, H^2_+$. Here

$$\mathbf{S}_{LPh} = S^+(p) = S^{-1}(p) = S^+_\beta(\lambda) = \frac{ip + \beta_{00} - \beta_{01}\,\beta^{-1}_{11}\,\beta_{10} - \beta_{01}\,\beta^{-1}_{11}\left[Trace\ \frac{1+A^2}{\lambda I - A}P_i\right]^{-1}\ \beta_{10}}{ip - \beta_{00} + \beta_{01}\,\beta^{-1}_{11}\,\beta_{10} + \beta_{01}\,\beta^{-1}_{11}\left[Trace\ \frac{1+A^2}{\lambda I - A}P_i\right]^{-1}\ \beta_{10}}. \tag{87}$$

is the Lax-Phillips scattering matrix of the string, represented by the finite Blashke-product, see [30]. It is an analytic function in the upper half-plane with zeros at $p_s(\beta)$. It also serves the characteristic function of the Lax-Phillips semigroup obtained via restriction of the unitary evolution group $e^{i\mathcal{L}_\beta} \to P_K\ e^{i\mathcal{L}_\beta}\ P_K,\ t \geqslant 0$ onto the inner space $K =: E_A \oplus E_A$, obtained as an orthogonal complement of the incoming and outgoing waves in the wires, see [30], where , in particular, the acoustic scattering problem is studied on the string without the inner hamiltonian attached. Being a characteristic function of a contracting semigroup, the Lax-Phillips Scattering matrix admits a factorization into the product of a pair of factors corresponding to invariant subspaces of the Lax-Phillips semigroup, for instance as a product of the Blashke-factor containing $p_1(\beta)$ and the complementary product extended on $s = 2, 3, \ldots$. The corresponding factorization is valid also for

$$\mathbf{S}^\beta = \mathbf{S}_1^\beta(p)\ \mathbf{S}_\beta^1(p) = -\frac{[p + p_1(\beta)]\,[p - \bar{p}_1(\beta)]}{[p + \bar{p}_1(\beta)]\,[p - p_1(\beta)]}\ \prod_{s \neq \pm 1} \frac{p - \bar{p}_s(\beta)}{p - p_s(\beta)}. \tag{88}$$

The "resonance" factor of the scattering matrix, taking into account both resonance zeros $\bar{p}_1(\beta), -p_1(\beta)$ approaching $\pm p_1(0) = \pm\alpha_1$, is non-analytic at the origin in the $[\beta_{01}]^{-1}$-plane, when $p$ is close to $\pm\alpha_1$, due to above reason, but the complementary factor of the scattering matrix, is analytic with respect to $|\beta_{01}|^{-2}$ near the origin in $|\beta_{01}|^{-2}$ -plane, when $p$ is close to $\pm\alpha_1$.

**Theorem 6.2.** *There exists a one-dimensional perturbation $\mathbf{A}_1^\beta$ of the operator*

$$l_0 u = -u'',\ u\Big|_0 = 0$$

*with a non-trivial inner component, such that the scattering matrix of the pair $(\mathbf{A}_1^\beta, l_0)$ coincides with $\mathbf{S}_1^\beta(p)$. Then the scattering matrix of the complementary pair $(\mathbf{A}_\beta, \mathbf{A}_1^\beta)$ is equal to the complementary factor $\mathbf{S}_\beta^0(p)$ and the following chain-rule for the scattering matrices is true*

$$\mathbf{S}^\beta(p) = \mathbf{S}_1^\beta(p)\ \mathbf{S}_\beta^1(p),$$

*as well, as the corresponding chain rule for the inverse, which are Lax-Phillips Scattering matrices. The complementary factor is an analytic function of $[\beta^{-1}, p]$ on the product $(\Omega_\beta \times [\Omega_{\alpha_1} \cup \Omega_{-\alpha_1}]$ of a small neighborhood of the origin in $\beta_{01}$-space and a small neighborhood of the pair $-\alpha_1, \alpha_1)$ in the $p$-plane.*

*Proof*. Consider a one-dimensional operator $A$ with a positive eigenvalue $\alpha = \alpha^2(\beta)$, which will be specified later. We associate with $A$ the Krein function $\mathcal{M} = \frac{1+\alpha^2\lambda}{\alpha^2-\lambda}$, by setting $|P_i\nu| = 0$. Restrict the operator $l \to l_0$ onto functions vanishing at the origin $x = 0$, and construct the self-adjoint extension of $l_0$ with a one-dimensional exit from $L_2(R_+)$, defined by the $2 \times 2$ Hermitian matrix $\{\beta\}$ which connects the boundary values $\{\xi_+, \xi_-\} = \{\xi_+, -\mathcal{M}\xi_+\}$ in $E_A$ with boundary values $\Psi(0),\ \Psi'(0)$ in $E_+$:

$$\begin{pmatrix} \Psi' \\ -\xi_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta_{10} & \beta_{11} \end{pmatrix} \begin{pmatrix} \Psi \\ -\xi_- \end{pmatrix}. \tag{89}$$

Substituting into the above equation the corresponding Ansatz for the wave-function of the problem (76) in the outer space

$$\Psi_0^\beta(x, p) = e^{ipx} + \mathbf{S}^\beta(p) e^{-ipx}, \tag{90}$$

we obtain an explicit expression for the corresponding scattering matrix $\mathbf{S}$ in terms of the Krein function $\mathcal{M}(\lambda) = \frac{1+\alpha^2\lambda}{\alpha^2-\lambda}$ of the inner Hamiltonian and the boundary parameters:

$$\mathbf{S}_0^\beta(\lambda) = \frac{ip - \left[\beta_{00} - \frac{|\beta_{01}|^2\mathcal{M}}{1+\beta_{11}\mathcal{M}}\right]}{ip + \left[\beta_{00} - \frac{|\beta_{01}|^2\mathcal{M}}{1+\beta_{11}\mathcal{M}}\right]}.$$

Selecting the parameter $\beta_{11}$ such that $1 - \beta_{11}\alpha^2 = 0$, we get $1 + \beta_{11}\mathcal{M} = \frac{\beta_{11}+\alpha^2}{\alpha^2-\lambda}$, and obtain the scattering matrix with $\lambda = p^2 + \pi^2\delta^{-2} + V$ in the form (80) with $\alpha_r \equiv \alpha$

$$S_\beta(\lambda) = \frac{ip - \det\beta\beta_{11}^{-1} + \frac{|\beta_{01}|^2}{\beta_{11}}(1+\alpha^4)(p^2-\alpha^2)}{ip + \det\beta\beta_{11}^{-1} - \frac{|\beta_{01}|^2}{\beta_{11}}(1+\alpha^4)(p^2-\alpha^2)} =$$

$$\frac{ip - \left[\frac{\det\beta}{\beta_{11}} + \frac{|\beta_{01}|^2\,\alpha^2}{\beta_{11}\,(1+\alpha^4)}\right] + p^2\frac{|\beta_{01}|^2}{\beta_{11}\,(1+\alpha^4)}}{ip + \left[\frac{\det\beta}{\beta_{11}} + \frac{|\beta_{01}|^2\,\alpha^2}{\beta_{11}\,(1+\alpha^4)}\right] - p^2\frac{|\beta_{01}|^2}{\beta_{11}\,(1+\alpha^4)}}, \tag{91}$$

which is compatible with the first factor in (88)). Comparing the corresponding addenda of the denominators,

$$\mathbf{S}_0^\beta(p) = -\frac{[(p+p(\beta)]\,[p-\bar{p}(\beta)]}{[p+\bar{p}(\beta)]\,[p-p(\beta)]} = -\frac{p^2 + 2i\Im p(\beta)\,p - |p(\beta)|^2}{p^2 - 2i\Im p(\beta)p - |p(\beta)|^2},$$

we obtain equations for parameters $\beta_{01}, \beta_{00}$ of the extension $\mathbf{A}_0^\beta$:

$$\frac{1}{2\Im p(\beta)} = \frac{\frac{\det\beta}{beta_{01}} + \frac{|\beta_{01}|^2\,\alpha^2}{\beta_{11}(1+\alpha^4)}}{|p(\beta)|^2} = \frac{\frac{|\beta_{01}|^2\,\alpha^2}{\beta_{11}(1+\alpha^4)}}{1} \tag{92}$$

Assuming that $\beta_{11}\alpha^2 = 1$. we obtain , comparing the first and the third fractions

$$|\beta_{01}|^2 = \frac{\beta_{11}(1+\alpha^4)}{2\Im p(\beta)},$$

and recover $\beta_{00}$, based on that, from the second fraction:

$$\beta_{00} = \frac{|\beta_{01}|^2}{\beta_{11}}\left[1 - \frac{\alpha^2}{1+\alpha^4}\right] + \frac{|p(\beta)|^2}{2\Im p(\beta)}$$

The chain rule for scattering matrices can be obtained based on the interpretation of the scattering matrix as a characteristic function of the relevant Lax-Phillips semigroup [56] on the semi-axis for the acoustic equation $u_{tt} - u_{xx} = 0$, with the above boundary condition, with inner structure. According to fundamental results of [55] both inner factors of the factorization of the characteristic function are interpreted as characteristic functions of the Lax-Phillips semigroup on the corresponding invariant subspaces, hence - as scattering matrices of the complementary pairs of operators. One can also calculate the wave operators between the operators involved , see [56], and derive the chain rule for the Lax-Phillips scattering matrices (characteristic functions) from the standard chain rule for the wave operators, see more details in [57].

**Corollary.** Summarizing our observations we suggest, based on 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 $\beta^{-1}$, at the origin) scattering matrix. This scattering matrix is a factor of the complete scattering matrix, which contains the *dangerous resonances* approaching to the resonance eigenvalue of the Intermediate Hamiltonian and is an

exact factor of the complete scattering matrix, so that the division of the scattering matrix through the non-analytic factor yields an analytic with respect $\beta^{-1}$ remaining part.

b. Second step is the calculation of the remaining part of the scattering matrix of the model by the standard analytic perturbation procedure. Due to analyticity of the remaining part with respect to $\beta^{-1}$, the analytic perturbation procedure is converging, with the radius of converging defined by the spacing between the eigenvalues $\alpha_1^2,\ \alpha_s^2,\ s \neq 1$. The analytic factor is interpreted as the scattering matrix between the constructed kick-start solvable model and the perturbed operator $\mathbf{A}^\beta$.

The obtained connection between resonances and analytic perturbation series on the continuous spectrum is a spectral analog of the connection between small denominators in celestial mechanics and divergence of the perturbation series, observed by H. Poincaré, see [31]. More historical comments about intermediate Hamiltonian and the jump-start (kick -start) may be found in [37], where similar modification of the analytic perturbation procedure for the Friedrichs model is suggested.

Note that recovering of *exact* information on the resonance $p_\beta$ and on the corresponding residue for the perturbed operator $\mathbf{A}_\beta$, which we need to develop the "jump-start"(kick-start) procedure, may be a tricky problem - almost equivalent to the original spectral problem. On the other hand, if the *approximate* resonance factor $\mathbf{S}_0^\beta$ is used instead the the exact factor, then the division of the scattering matrix through $\mathbf{S}_0^\beta$ would not eliminate singularity at the resonance, hence the complementary factor of the scattering matrix would be still non-analytic at the origin in the space of the coupling constant, hence could not be obtained via analytic perturbation procedure.

### 6.2. Resonance pumping of the acoustic junction. The quantum version of the pumping

The Lax-Phillips interpretation of the scattering on the above simplest junction reveals the spectral nature of the poles of the Scattering matrix, or, equivalently, the zeros of the Lax-Phillips Scattering matrix: they are the eigenvalues of the generator of the Lax-Phillips semigroup

$$P_K e^{i\mathcal{L}t} P_K \equiv e^{i\mathcal{B}t},\ t \geqslant 0.$$

Thus the above kick-start analytic perturbation procedure permits to observe creation of resonances from the embedded eigenvalues of the unperturbed problem $A \oplus l_0$. The spectal properties of the generator $\mathcal{B}$ are easily established in Fourier representation $\mathcal{J}$, see [55]. In particular, the eigenvalues of the generators $\mathcal{B}$, $\mathcal{B}^+$ are the zeros and poles $p_s(\beta),\ \bar{p}_s(\beta)$ of $\mathcal{S}_{LPh}$, and the eigenfunctions of $\mathcal{B}$, $\mathcal{B}^+$ are, respectively, in the case of the simple eigenvalues:

$$\psi_s(p) = \frac{\mathbf{S}_{LPh}}{p - p_s(\beta)})\ \sqrt{\Im p_s(\beta)},\ \phi_s(p) = \frac{1}{p - \bar{p}_s(\beta)})\ \sqrt{\Im p_s(\beta)}.$$

They form a bi-orthogonal system in $K = H_+^2 \ominus \mathbf{S}_{LPh}\ H_2^2$. The spectral representation of the generator is, see [55],

$$\mathcal{B} = \sum_s p_s(\beta) \langle \phi_s(p), * \rangle\ \psi_s(p)\ \frac{1}{2\pi\, i\, \mathbf{S}'_{LPh}(p_s(\beta))} \tag{93}$$

Pumping of a junction with a periodic train of pulses

$$\frac{1}{i}\frac{\partial u}{\partial t} = \mathcal{B}u + e^{i\omega t} f,\ u, f \in K,\ u\Big|_{t=0} = u_0,$$

causes a linear growth of the amplitude of the resonance components of the oscillation process on the junction:

$$u = \sum_s u_s(t)\,\psi_s,\ \text{where}\ u_s(t) = u_s(0)\,e^{ip_s\,t} + \frac{e^{i\omega t} - e^{ip_s t}}{\omega - p_s}\ f_s \approx u_s(0)\,e^{ip_s\,t} + t\ f_s, \tag{94}$$

if $\omega = \Re p_s$ and $\Im p_s$ is Schrödinger evolution on the inner subsystem is described, in terms of Lax-Phillips representation $J_{\mathcal{E}}$ by the family of operators $P_K\,e^{ip^2\,t}P_K$, which is not a semigroup, contrary to the case of the wave equation with $P_K\,e^{ip^2\,t}P_K$ substituted by the semigroup $P_K\,e^{ipt}P_K,\ t > 0$. One usually represent $P_K\,e^{ip^2\,t}P_K$ as a sum of the contribution from the terms corresponding to resonances situated below the bisectrix $\Gamma$ of the first quadrant $0 < \Re p_s < \Im p_s$, and the contribution represented, in x-representation , by the Gaussian integral $\frac{1}{2\pi}\int_\Gamma P_K\mathbf{\Psi}e^{ip^2\,t}J_{\mathcal{E}}\vec{\mathbf{U}}$ , which is estimated, for large $t$, by the contribution $O(1/t)$ from the point $p = 0$ on the contour. This non-exponenial decay of the Schrödinger evolution on the inner subsystem was discovered theoretically long ago, see , [58], but was not confirmed by experiments since that. This gives a good reason to represent the portion of the Schrödinger evolution in the inner subsystem by the contribution from resonances situated below the bisectrix. In Lax-Phillips representation this contribution looks like

$$J_{\mathcal{E}}\vec{\mathbf{U}}_{inner} = \sum_{0<\Re p_s<\Im p_s} e^{ip_s^2\,t}\psi_s\rangle\,\langle\phi, J_{\mathcal{E}}\vec{\mathbf{U}}\rangle. \tag{95}$$

Here the non-exponential decay is neglected. The question on estimation of the non-exponential decay in agreement with experiment is not resolved yet theoretically. But if we base an estimation of the quantum resonance pumping on the above formula, then the effect of the periodic train of waves $e^{i\omega t}f$, with the resonance frequency $\omega = \Re p_s^2$ gives the quantum analog of the above formula (94)

$$u = \sum_s u_s(t)\,\psi_s,\ \text{where}\ u_s(t) = u_s(0)\,e^{ip_s^2\,t} + \frac{e^{i\omega t} - e^{ip_s^2 t}}{\omega - p_s^2}\ f_s \approx u_s(0)\,e^{ip_s^2\,t} + t\ f_s, \tag{96}$$

with summation extended over resonances situated below the bisectrix of the first quadrant.

## 7. Appendix. Matrix Rouche theorem

Let $E_0$ be a proper subspace of the finite-dimensional Hilbert space $E$ , $P_0$ is an orthogonal projection onto $E_0$ and $P_0^\perp = I - P_0$ - the complementary projection onto the orthogonal complement $E_0^\perp = E \ominus E_0$. We say that the analytic matrix-function $m$ has an *simple isolated vector zero* at the point $\mu_0 \in D_m$ if it may be represented in a neighborhood $U_0 \subset D_\mu$ as a product

$$m(\mu) = m_0(\mu)\left[(\mu - \mu_0)P_0 + bP_0^\perp\right] \tag{97}$$

with some nonzero constant $b$ and an invertible analytic matrix-function $m_0(\mu)$

$$m_0(\mu) = m_0(\mu_0) + \frac{\mu - \mu_0}{1!}m_0'(\mu_0) + \ldots,\ \text{Ker}\ m_0(\mu_0) = 0.$$

The vectors $\{e_0\} \in E_0$ are called *root-vectors*, $m(\mu_0)e_0 = 0$. For vectors $e_\perp$ from the complementary subspace $e_\perp \in E_{0\perp}$ we have $m(\mu_0)e_\perp \neq 0$ . Similarly the *simple isolated vector pole* is defined: we say that the function $m$ has a simple isolated vector pole at the point $\mu_0$ if it is represented as

$$m(\mu) = m_0(\mu)\left[\frac{P_0}{\mu - \mu_0} + bP_0^\perp\right] \tag{98}$$

with a non-zero constant $b$ and a projection $P_0$ onto proper subspace $E_0 \subset E$, the complementary projection $P_0^\perp$ and an analytic invertible function $m_0$ in a neighborhood $U_0$ of the point $\mu_0$ in

$D_m$. Both isolated poles and zeroes of analytic matrix-functions are called in [45] *characteristic values* of the argument $\mu$.

The logarithmic residue of the function $\mu$ at the simple isolated zero or pole is defined as an integral of the logarithmic derivative $m'(\mu)m^{-1}$ on a simple smooth curve $\Gamma_0 \subset U_0$ in anti-clockwise ("positive") direction around the characteristic value $m_0$:

$$I_{m,\mu_0} = \frac{1}{2\pi i}\oint_{\Gamma_0} m'(\mu)m^{-1}d\mu.$$

In [45] the *period* of the logarithmic derivative $m'(\mu)m^{-1}$

$$m_{m,\mu_0} = \frac{1}{2\pi i}Trace\oint_{\Gamma_0} m'(\mu)m^{-1}d\mu.$$

is called the "multiplicity"of the characteristic value. The straightforward calculation of above integrals gives the following result:

$$I_{m,\mu_0} = \frac{1}{2\pi i}\oint_{\Gamma_0} m'(\mu)m^{-1}d\mu =$$

$$\frac{1}{2\pi i}\oint_{\Gamma_0} m_0(\mu)P_0\left[(\mu_0-\mu)P_0+bP_0^{\perp}\right]^{-1}m_0^{-1}(\mu)(\mu)d\mu =$$

$$\frac{1}{2\pi i}m_0\mu_0\oint_{\Gamma_0} P_0\left[(\mu_0-\mu)P_0+bP_0^{\perp}\right]^{-1}d\mu m_0^{-1}(\mu_0) = m_0\mu_0P_0m_0^{-1}(\mu_0),$$

and

$$M_{m,\mu_0} = \pm\mathrm{dim}P_0,$$

where the sign $\pm$ is defined by the sort of the characteristic value: plus is for the zero, and minus is for the pole. We will use the "hermitian" variant of the Gohberg-Sigal theorem, assuming that all poles (zeroes)are simple (first order):

**Theorem 7.1.** *If two finite square matrices $m_s(\mu)$, $s = 0, 1$ depend analytically on the parameter $\mu$ in the disc $D$ radius $\tilde{\delta}$ centered at the point $\mu = \tilde{\alpha}_0$, and $m_0$ has few characteristic points $\mu_0^s$ inside the disc $D_0 = \left\{\mu : |\mu - \tilde{\alpha}_0| \leqslant 1/2\ \tilde{\delta}_0 < 1/2\ \tilde{\delta}\right\}$ with the total multiplicity*

$$M_0 = \sum_s M_0^s,$$

*and on the circle $\Sigma_0 = \left\{\mu : |\mu - \tilde{\alpha}_0| =\leqslant 1/2\ \tilde{\delta}_0\right\}$ both functions have no characteristic values and the inequality*

$$max_{\mu\in\Sigma_0} \parallel m_0^{-1}(\mu)\left[M_1(\mu) - M_0(\mu)\right] \parallel < 1$$

*is fulfilled, then the total multiplicity $M_1$ of characteristic values of the function $m_1$ inside the circle $\Sigma_0$ is equal to total multiplicity $M_0$ of the characteristic values of the function $m_1$.*

Proof of much more general statement concerning analytic functions with multiple poles and zeroes may be found in [45]. We actually need in the above text , section 3, a partial statement concerning the case when both functions are regular and $M_0 = 1$. Then $m_1$ has a single simple isolated zero inside the disc $\Sigma_0$. The case of a single pole may be reduced to the case of a single zero via considering inverse functions.

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