Modified Krein formula, analytic perturbation procedure and a solvable model of an arbitrary junction

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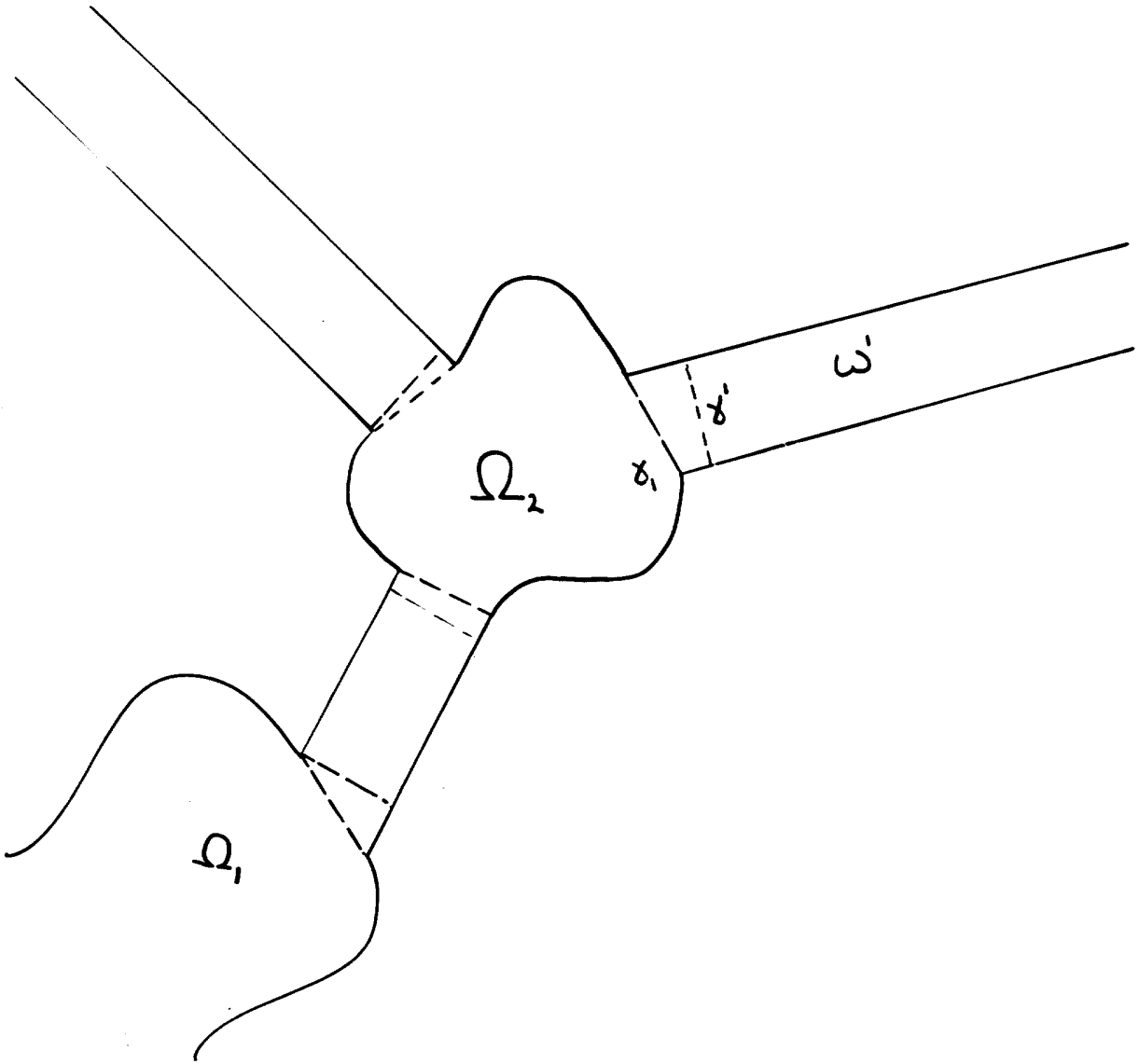
Introduction

- Quantum Network is constructed of the vertex domains (quantum wells Ω_s) and straight leads (quantum wires ω^m), of equal width δ connecting the wells to each other or extending to infinity. It is convenient to assume, that the domains and the leads are separated from each other by imaginable orthogonal bottom sections $\gamma_m,\ \cup_m \gamma_m = \Gamma$. The dynamic of a single 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 for the Schrödinger operator $\mathcal{L}$ on the network.

Introduction



Quantum Network - a detail.

Introduction

- $$\mathcal{L}\psi = -\triangle\psi + \mathsf{V}\psi = \lambda\psi,$$

  The potential V is a real constant V_δ on the wires and it is a piecewise continuous function V_s on the wells Ω_s. We consider hereafter a star shaped network Ω- *a junction*- with a single well Ω_{int} and few quantum wires ω^n attached to it, and denote by $\Omega\backslash\Omega_{int} := \cup_n\, \omega^n =: \omega$ – the "exterior part" of the network.

Introduction

- Theoretical analysis of the electron transport problem in the junction is usually reduced to one-electron scattering problem, see [1-3] for the pair of Hamiltonians: the one-electron Schrödinger operator $\mathcal{L}$ on the junction and the splitting of it $\mathcal{L} \to L_{int} \oplus l^{\omega} := \mathcal{L}_0$ of it into orthogonal sum of $L_{int} = \mathcal{L}|_{L_2(\Omega_{int})}$ and $l^{\omega} = \mathcal{L}|_{L_2(\omega)}$, obtained via imposing of additional zero boundary condition on Γ- a "solid wall". The part l^{ω} of the split operator plays a role of a standard unperturbed Hamiltonian in the above scattering problem.

Introduction

- This scattering problem is a sophisticated perturbation problem for the operator $\mathcal{L}_0$ which has embedded eigenvalues. Under the perturbation - removing the solid wall on Γ- the standing waves in the vertex domain Ω_{int} are bred with the running waves in the wires, resulting in resonances which define the resonance character of the transmission across the junction. Analytical calculation of the scattering matrix of the two-dimensional junction is a difficult mathematical problem. For practical needs the physicists substitute the junction by a quantum graph, with an appropriate boundary condition at the vertex, see [1-3].

Introduction

- Validity of that solvable model was confirmed via smooth approximation of the graph by thin manifold shrinking to the graph, see for instance [4,5]. This analysis showed, in particular for uniform shrinking, that the eigenvalues, *at the lower spectral threshold*, $\lambda = 0$, of the two-dimensional Schrödinger equation on the manifold - the "fattened graph", with Neumann boundary conditions, - converge to the eigenvalues of the one-dimensional Schrödinger equation on the graph, with the Kirchhoff boundary condition at the vertex a : $\sum_s \frac{d\psi_s}{dx}(a) = 0$. This result is proved in [5]. In fact scattering of electrons in quantum networks is observed on the small, for low temperature, essential spectral interval centered at the Fermi level. Validity of the Kirchhoff boundary condition for electrons on the Fermi level in the quantum network is questioned in [6].

Introduction

- In [7], see also references therein, the resonance mechanism of conductance across the junction is considered. For thin junction the role of main detail of the transmitting mechanism is played by the resonance eigenfunction φ_0 on the junction, which corresponds to the eigenvalue λ_0 closest to the Fermi - level L_0. The magnitude of the transmission coefficient is defined by the shape of the resonance eigenfunction of the Schrödinger operator on the vertex domain of the junction. This mechanism permits to interpret the phenomenological parameter in the boundary condition suggested by Datta [1] for T-junction.

Introduction

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

Scattering in Quantum Networks

- The scattering problem on the junction is reduced to comparison spectral characteristics of $\mathcal{L}$ with ones of the split operator $\mathcal{L}_0$.
  The spectrum $\sigma(L_{int})$ of L_{int} is discrete, and the spectrum $\sigma(l^\omega)$ of l^ω is absolutely continuous. It consists of spectral branches
  $$\sigma^r = [\frac{\pi^2 r^2}{\hbar^2}, \infty),\ r = 1, 2, \dots$$
  and can be represented as a countable sum of spectral bands
  $$\Delta_r = [\frac{\pi^2 r^2}{\hbar^2}, \frac{\pi^2 (r+1)^2}{\hbar^2}],\ \ r = 1, 2, \dots,$$
  separated by the thresholds $\frac{\pi^2 r^2}{\hbar^2}$. The spectral band containing the scaled Fermi level $\Lambda^F := \frac{2 m_0 \kappa T}{\hbar^2}$ is called the conductivity band.

Scattering in Quantum Networks

- The components Ψ^r of the eigenfunctions Ψ of l^ω- partial scattered waves- are spanned by the cross-section eigenfunctions of the wires $e_r^\omega = \sqrt{2/\delta}\sin\frac{\pi r x^\perp}{\delta}$, $E_r = \bigvee_\omega e_r^\omega,\ 0 < x^\perp < \delta, \lambda \in \sigma^r, r = 1, 2, \dots$:

$$\Psi^r(x^\parallel, x^\perp) = \sin\sqrt{\lambda - [\frac{\pi^2 r^2}{\delta^2} + V_\delta]x^\parallel}\ e_r,\ 0 < x^\parallel < \infty.$$

The channels $\mathcal{H}_r \subset L_2(\omega)$

$$\mathcal{H}_r = L_2(0, \infty) \times E_r$$

are invariant subspaces of $l^\omega = \oplus_r l^r$, $\sigma(l^r) = \sigma_r$. We call E_r the entrance subspaces of the channels $\mathcal{H}_r \subset L_2(\omega)$.

Scattering in Quantum Networks

- For given temperature T we consider an essential spectral interval Δ_T:

$$\Delta_T := \left(\Lambda_F - \frac{2m\,\kappa T}{\hbar^2}, \Lambda_F + \frac{2m\,\kappa T}{\hbar^2} \right),$$

centered at the scaled Fermi level $\frac{2m\,E_F}{\hbar^2} =: \Lambda^F =: \Lambda$. If the temperature is low, $\Delta_T := \Delta$ is contained inside the conductivity band: there are no spectral thresholds inside Δ.

Scattering in Quantum Networks

- One - body transport problem for the quantum network is solved, if the scattered waves of $\mathcal{L}$ are constructed. The scattered waves are obtained via matching on Γ of solutions of the Schrödinger equation $L\psi = \lambda\psi$ in Ω_{int} with the scattering Ansatz $\vec{\psi}(x,\lambda) = \left\{\psi_l^m(x,\lambda)\right\}$ in the wires $\omega^m = (x : 0 < x^{\|} < \infty,\ 0 < x^{\perp} < \delta)$. The Ansatz is combined of oscillating modes, or exponentially decreasing modes in the open $(\Lambda - V_\delta - \pi^2 l^2 \delta^{-2} > 0)$ and closed $(\pi^2 l^2 \delta^{-2} + V_\delta - \Lambda > 0)$ channels in the wires respectively, for given scaled Fermi level Λ:

Scattering in Quantum Networks

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

  $$\xi^{I}(x) := \exp\left(-\sqrt{\pi^2 I^2 \delta^{-2} + V_\delta - \lambda}\; x^{\parallel}\right)\; e_I(x^{\perp}).$$

  Then the scattering Ansatz on Δ_T is

Scattering in Quantum Networks

$$\psi_l^m(x) =$$

$$\begin{cases} \chi_+^l(x) + \sum_{open,r} S_{l,r}^{m,m} \chi_-^r(x) + \sum_{closed,r} s_{l,r}^{m,m} \xi^r(x), x \in \omega^m \\ \sum_{open,r} S_{l,r}^{m,n} \chi_-^r(x) + \sum_{closed,r} s_{l,r}^{n,m} \xi^r(x), x \in \omega^n,\ n \neq m. \end{cases} \quad (1)$$

We introduce the entrance spaces of open and closed channels

$$E_+ = \oplus \bigvee_{open,r} E_r,\ E_- = \oplus \bigvee_{closed,r} E_r$$

and the channel spaces $\mathcal{H}_\pm = E_\pm \times L_2(0,\infty)$ - the invariant subspaces of $I^{out} := \mathcal{L}|_{L_2(\omega)}$ corresponding to the open and closed branches of the continuous spectrum.

Scattering in Quantum Networks

- Matching on Γ of the scattering Ansatz $\vec{\psi}$ to the solution of the Schrödinger equation inside the quantum well Ω_{int} gives an infinite linear system for the coefficients S^n_{lr}, s^n_{lr}, see [1]. Indeed, according to general theory of second order linear equations, see [2], the solution u of the boundary problem with data $u\Big|_\Gamma = u_\Gamma$ is represented by the integral map with the Poisson kernel:

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

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

Scattering in Quantum Networks

- Denoting by $K_\pm$ the exponents of the above Ansatz in the open and closed channels in the wires and by S, s the coefficients in front of the corresponding exponentials, we represent the Ansatz for the scattered wave in the wires, with $x^{\|} := x$:

$$\Psi(x,\nu) = e^{iK_+x}\,\nu + e^{-iK_+x}\,S\nu + e^{-K_-x}\,s\nu. \qquad (2)$$

Substitution of the Ansatz into the formula for DN-map gives an infinite linear system for the coefficients S, s. This system can be simplified via elimination "evanescent waves" with the coefficient s. This gives the Krein formula for the Scattering matrix similar to the corresponding one-dimensional formula,[10] used in modern approach to inverse problem, see [11]:

$$S(\lambda) = \frac{ik - m(\lambda)}{ik - m(\lambda)}$$

Scattering in Quantum Networks

- Our nearest aim is: to derive a two-dimensional analog of the above formula, with Weyl function m replaced by the Dirichlet-to-Neumann map [12] of an appropriate operator. The approximate scattering matrix is obtained via substitution of the Dirichlet-to-neumann map by certain rational approximation on an essential spectral interval centered at the scaled Fermi level. The formal boundary condition corresponding to the solvable model, is generally, energy-dependent. For low temperature it is reduced to Datta-type boundary condition with a projection defined by the boundary current of the resonance eigenfunction of the Intermediate Hamiltonian, see below.

Krein formula for the scattering matrix

- We achieve that by derivation a modified Krein formula for the Scattering matrix of the junction and developing a relevant analytic perturbation procedure based on the scattering matrix of the solvable model. Krein-type formula for the scattering matrix of a solvable model is derived in [13]. We will derive similar formula for the scattering matrix of a quantum network, which defines the resonance character of transmission across the junction on the essential spectral interval, centered at the Fermi level. For thin network the leading term of the approximate formula coincides with the solvable model of the network in form of a quantum graph with a resonance vertex, see [14].

Krein formula for the scattering matrix

- So: our aim is not the same as the aim of previous papers [4,5] but different one: we calculate the transport characteristics of an arbitrary junction and construct the corresponding solvable model [14], if the junction is thin. The model is fitted based on the data of the spectral analysis of the Schrödinger operator on the vertex domain, with Dirichlet boundary condition.

Krein formula for the scattering matrix

- The Krein formula for the scattering matrix, of the 2-d network is based on decomposition of the cross-section subspace $E := L_2(\Gamma) = E_+ \oplus E_-$. Consider the matrix representation of the DN-map of L_{int} with respect to the orthogonal decomposition and the corresponding projections $I = P_+ \oplus P_-$:

$$\mathcal{DN} = \begin{pmatrix} P_+\mathcal{DN}P_+ & P_+\mathcal{DN}P_+ \\ P_-\mathcal{DN}P_+ & P_-\mathcal{DN}P_- \end{pmatrix} := \begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}+- \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix}. \tag{3}$$

Krein Formula for the scattering matrix

- Comparing the Cauchy data of the scattering Ansatz on the bottom sections Γ

$$\Psi(\nu)\Big|_{\Gamma} = (I+S)\nu + s\nu,$$

$$\Psi'(\nu)\Big|_{\Gamma} = iK_{+}(I-S)\nu - K_{-}s\nu, \tag{4}$$

we are able to eliminate s from the equation

$$\mathcal{DN}\{[I+S]\nu + s\nu\} =$$

$$= iK_{+}[I-S]\nu - K_{-}s\nu,$$

Krein Formula for the scattering matrix

- and obtain the following formula for the scattering matrix, with the denominator preceding the numerator:

$$S = \frac{iK_+ - \left[\mathcal{DN}_{++} - \mathcal{DN}_{+-}\frac{I}{\mathcal{DN}_{--}+K_-}\mathcal{DN}_{-+}\right]}{iK_+ + \left[\mathcal{DN}_{++} - \mathcal{DN}_{+-}\frac{I}{\mathcal{DN}_{--}+K_-}\mathcal{DN}_{-+}\right]} \tag{5}$$

Krein Formula for the scattering matrix

- The expression

$$\mathcal{DN}_{++} - \mathcal{DN}_{+-}\frac{I}{\mathcal{DN}_{--} + K_-}\mathcal{DN}_{-+} := \mathcal{DN}^F \qquad (6)$$

has a structure typical for the classical Krein formula and can be interpreted as Dirichlet-to-Neumann map of an *Intermediate Hamiltonian*, see [6,15].
The Intermediate Hamiltonian L_F is introduced via splitting of $\mathcal{L}$ by the "partial" zero boundary condition imposed on Γ onto elements from the domain of $\mathcal{L}$:

$$P_+ u\Big|_\Gamma = 0. \qquad (7)$$

The original operator $\mathcal{L}$ is split by (7), $\mathcal{L} \longrightarrow L_F \oplus I^F$, into an orthogonal sum of two self-adjoint operators: the restriction I^F of $\mathcal{L}$ onto $\mathcal{H}_+$, and the restriction L_F of $\mathcal{L}$ onto $L_2(\Omega) \ominus \mathcal{H}_+$.

Krein Formula for the scattering matrix

- The orthogonal complement of the subspace of open channels consists of the invariant subspace of the closed channels in the wires and $L_2(\Omega_{int})$. Elements from the domain of L_F fulfil smooth matching condition on Γ in all closed channels. Though the operator L_F is not defined on the whole space $L_2(\Omega)$, but only on the subspace $L_2(\Omega) \ominus E_+$, yet the resolvent of it restricted as $(L_F - \lambda I)^{-1} : L_2(\Omega) \to L_2(\Omega_{int})$ is represented by an integral operator with the kernel $G^F(x, x'),\ x \in \Omega_{int},\ \ x' \in \Omega$. Then the corresponding Poisson kernel can be defined on Γ as $\frac{\partial G^F}{\partial n_\gamma}(x, \gamma)$.

The Intermediate Hamiltonian

- The solution of the intermediate boundary problem

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

is obtained via the Poisson formula

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

$$\frac{\partial u(x)}{\partial n}\bigg|_\Gamma = -\int_\Gamma \frac{\partial^2 G^F}{\partial n\, \partial n_\gamma}(x,\gamma)\ u_+ d\Gamma,\ x \in \Gamma.$$

The Intermediate Hamiltonian

- Then

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

  which implies the standard formula for DN-map of L_F

$$P_+ \frac{\partial u_+}{\partial n_\gamma}\bigg|_\Gamma := \mathcal{DN}^F u_+. \tag{8}$$

The Intermediate Hamiltonian

- Due to introduction of the intermediate Hamiltonian we are able to re-write the formula (5) for the scattering matrix in more compact form

$$S(\lambda) = \frac{iK_+ - \mathcal{D}\mathcal{N}^F}{iK_+ - \mathcal{D}\mathcal{N}^F}, \tag{9}$$

with the denominator preceding the numerator. Now this formula looks similar to the corresponding one-dimensional formula. One may hope that the above formula may play a role in inverse problems for two-dimensional and multi-dimensional quantum networks

Analytic perturbation procedure for Krein denominator.

- Both terms in the left side of (6) have singularities on the spectrum of the non-perturbed operator L_{int}. In fact the singularities of the first and second term at the eigenvalues of L_{int} compensate each other, so that only the zeros of the denominator arise as singularities of the whole expression for DN-map of the intermediate Hamiltonian L_F. When observing the compensation of singularities we will obtain an explicit equation for the eigenvalues of the Intermediate Hamiltonian and calculate the residues at the corresponding poles of the intermediate DN-map.

Analytic perturbation procedure for Krein denominator.

- We assume that the temperature is *low*, so that the essential spectral interval is situated inside the conductivity band between the lower threshold λ_{min} of the closed channels and the upper threshold λ_{max} of the open channels:

$$\Delta_T \subset (\lambda_{max}, \lambda_{min}) .$$

  Our aim is: to construct a rational approximation of the DN-map of the intermediate Hamiltonian. But simultaneously we will suggest a semi-analytic method for construction of a convenient approximation for the Scattering matrix of any junction.

Analytic perturbation procedure for Krein denominator.

- Represent the DN-map $\mathcal{DN}$ of L_{int} on the essential spectral interval as a sum

$$\mathcal{DN} = \mathcal{DN}^{\Delta_T} + \mathcal{K} \tag{10}$$

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

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

Analytic perturbation procedure for Krein denominator.

- Due to the spectral representation of the $\mathcal{DN}$, see [4], we have

$$\mathcal{DN}_{+-}^{\Delta_T} = \sum_{\lambda_s \in \Delta_T} \frac{P_+ \frac{\partial \varphi_s}{\partial n} \rangle \langle P_+ \frac{\partial \varphi_s}{\partial n}}{\lambda - \lambda_s}, \tag{11}$$

where φ_s are the eigenfunctions of L_{int} on Δ_T. We introduce also the linear hull $E^{\Delta_T} = \bigvee_s \{\varphi_s\}$ - an invariant subspace of L_{int} corresponding to the essential spectral interval Δ_T and the part $L^{\Delta_T} := \sum_{\lambda_s \in \Delta_T} \lambda_s \varphi_s \rangle \langle \varphi_s$ of L_{int} in the invariant subspace E^{Δ_T}.

Analytic perturbation procedure for Krein denominator.

- To calculate the intermediate DN-map

$$\mathcal{DN}^F g = \mathcal{DN}_{++} g - \mathcal{DN}_{+-} \frac{I}{\mathcal{DN}_{--} + K_-} \mathcal{DN}_{-+} g \qquad (12)$$

in terms of the standard DN - map of L_{int} we have to solve the equation:

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

on the essential spectral interval Δ_T. *We are able to do that if K_- can play a role of a large parameter, so that the operator*

$$[\mathcal{K}_{--} + K_-]^{-1} \qquad (13)$$

exists on Δ_T.

Analytic perturbation procedure for Krein denominator.

- Using the above large parameter, we are able to develop an analytic perturbation procedure for the denominator in the Krein formula. Denote by T the map

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

and introduce

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

and

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

Compensation of singularities.

- The perturbation procedure permits to observe the compensation of singularities in Krein formula for $\mathcal{DN}^F$ inherited from L_{int}

  Theorem on compensation of singularities *If the condition (13) is fulfilled on the essential spectral interval* Δ *then the intermediate DN-map can be represented on* Δ *as*

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

$$-\mathcal{K}_{+-}\frac{I}{\mathcal{K}_{--}+K_-}\mathcal{K}_{-+} + P_+\mathcal{J}T^+\rangle\frac{I}{\lambda I - L^{\Delta_T} + Q(\lambda)}\langle T\mathcal{J}^+P_+. \tag{14}$$

  We call the above representation (14) **the modified Krein formula** for DN- map. Similar formula, with compensated singularities, can be derived based on Lippmann-Schwinger equation or from the corresponding Birman-Schwinger representation for its solution.

Intrinsic large parameter and analytic perturbation procedure

- The scattering matrix of the original problem on the essential spectral interval may be obtained via replacement of the intermediate DN-map in (5) by the expression (14) with compensated singularities. This substitution is possible for thin junctions, when the exponent K_- in closed channels can play a role of a large parameter, compared with the error $\mathcal{K}_{--}$ of the rational approximation $\mathcal{DN}^{\Delta_T}$ of $\mathcal{DN}$. This condition may be not satisfied for given Fermi level $\Lambda := \Lambda_0$.

Intrinsic large parameter and analytic perturbation procedure.

- In fact the choice of the "technical" Fermi level $\Lambda^F := \Lambda_0$ is in our hands, so we are able to select another value $\Lambda_1 >> \Lambda_0$, such that the condition (13) is fulfilled. The corresponding splitting of the original Hamiltonian would be defined by the orthogonal decomposition of the entrance space $E = \left[E_+^0 \oplus E_+^1\right] \oplus E_-^1$, such that few closed channels with thresholds $V_\infty + \frac{\pi^2 l^2}{\delta^2}$ situated between Λ_0 and Λ_1 are formally included into the lower group of channels, with an extended entrance subspace $E_+^0 \oplus E_+^1 := E_+$. We will use hereafter the intermediate DN-map $\mathcal{DN}^1$ of the operator L_1, defined by the semi-transparent boundary condition *hight* Λ_1 associated with the above decomposition of the entrance space $L_2(\Gamma) = \left[E_+^0 \oplus E_+^1\right] \oplus E_-^1$.

Intrinsic large parameter and analytic perturbation procedure.

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

  Denote by $K^0_+, K^1_\pm$ the exponents of the oscillating and decreasing solutions of the Schrödinger equation in the channels associated with E^0_+, $E^1_\pm$,respectively. Consider the orthogonal decomposition $E = E^0_+ \oplus E^1_+ \oplus E^1_-$ and represent the DN-map $\mathcal{DN}$ of L_{int} by the matrix

$$\mathcal{DN} = \begin{pmatrix} \mathcal{DN}^{00}_{++} & \mathcal{DN}^{01}_{++} & \mathcal{DN}^{01}_{+-} \\ \mathcal{DN}^{10}_{++} & \mathcal{DN}^{11}_{++} & \mathcal{DN}^{11}_{+-} \\ \mathcal{DN}^{10}_{-+} & \mathcal{DN}^{11}_{-+} & \mathcal{DN}^{11}_{--} \end{pmatrix} := \mathbf{DN}. \qquad (15)$$

Intrinsic large parameter and analytic perturbation procedure.

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

$$\mathcal{DN} = \mathcal{DN}_\Delta + \mathcal{K},$$

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

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

Intrinsic large parameter and analytic perturbation procedure.

- We use hereafter appropriate notations for matrix elements, of the above decomposition of the DN-map:

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

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

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

Intrinsic large parameter and analytic perturbation procedure.

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

$$\sup_{\lambda \in G_\Delta} \| \mathcal{K}^{00}_{+-}(\lambda) \| < \sqrt{\Lambda_1^F - \Lambda^F - 2\mu^* \kappa T \hbar^{-2}}. \qquad (16)$$

Intrinsic large parameter and analytic perturbation procedure.

- If Λ_1 is defined from (16), we construct the corresponding decomposition $E = E_+ \oplus E_-$, with $E_+ = \left[E_+ \oplus E_+^1\right],\ E_- = E_-^1$

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

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

$$\mathcal{L} = L_F^1 \oplus l_1^F, \tag{17}$$

obtained by imposing on Γ the additional boundary condition

$$P_+ u\Big|_\Gamma = 0,$$

with $P_+ = P_+^0 \oplus P_+^1$.

Scattering matrix on the essential spectral interval.

- Note that the trivial part I_1^F of this splitting contains additional channels in the "lover" group of channels : $E_+ = E_+^0 \oplus E_+^1$, which rise to exponentially decreasing modes $e^{-K_+^1 x}\nu$. The matrix (15) connects the boundary data $\Psi(0)$, $\Psi'(0)$ of the scattering Ansatz

$$\Psi(x,\lambda) = e^{iK_+x}\nu + e^{-iK_+x}S\nu + e^{-K_+^1 x}s_+^1\nu + e^{-K_-^1 x}s_-^1\nu, \quad (18)$$

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

Scattering matrix on the essential spectral interval.

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

$$s^1_-\nu = \frac{I}{\mathcal{DN}^{11}_{--} + K^1_-}\left[\mathcal{DN}^{01}_{-+}(\nu + S\nu) + \mathcal{DN}^{11}_{-+}s^1_+\nu\right]$$

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

$$\begin{pmatrix} iK^0_+(\nu - S\nu) \\ -K^1_+ s^1_+\nu \end{pmatrix} = \tilde{\mathbf{DN}} \begin{pmatrix} (\nu + S\nu) \\ s^1_+\nu \end{pmatrix}.$$

Scattering matrix on the essential spectral interval.

- Here

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

where

$$\tilde{\mathcal{DN}}^{00}_{++} = \mathcal{DN}^{00}_{++} - \mathcal{DN}^{01}_{+-} \frac{I}{\mathcal{DN}^{11}_{--} + K^{1}_{-}} \mathcal{DN}^{10}_{-+},$$

$$\tilde{\mathcal{DN}}^{01}_{++} = \mathcal{DN}^{01}_{++} - \mathcal{DN}^{01}_{+-} \frac{I}{\mathcal{DN}^{11}_{--} + K^{1}_{-}} \mathcal{DN}^{11}_{-+},$$

Scattering matrix on the essential spectral interval.

$$\tilde{\mathcal{DN}}^{10}_{++} = \mathcal{DN}^{10}_{++} - \mathcal{DN}^{11}_{+-}\frac{I}{\mathcal{DN}^{11}_{--} + K^1_-}\mathcal{DN}^{10}_{-+},$$

$$\tilde{\mathcal{DN}}^{11}_{++} = \mathcal{DN}^{11}_{++} - \mathcal{DN}^{11}_{+-}\frac{I}{\mathcal{DN}^{11}_{--} + K^1_-}\mathcal{DN}^{11}_{-+}.$$

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

$$S(\lambda) = \frac{iK_+ - \left[\tilde{\mathcal{DN}}^{00}_{++} - \tilde{\mathcal{DN}}^{01}_{++}\frac{I}{\tilde{\mathcal{DN}}^{11}_{++}+K^1_+}\tilde{\mathcal{DN}}^{01}_{++}\right]}{iK_+ + \left[\tilde{\mathcal{DN}}^{00}_{++} - \tilde{\mathcal{DN}}^{01}_{++}\frac{I}{\tilde{\mathcal{DN}}^{11}_{++}+K^1_+}\tilde{\mathcal{DN}}^{01}_{++}\right]} \qquad (19)$$

Scattering matrix on the essential spectral interval.

- The ultimate representation (19) of the scattering matrix is completely finite-dimensional, hence convenient for computational process. The large parameter Λ_1 permits to eliminate the infinite-dimensional part K_-^1 of K_- and obtain a completely finite-dimensional formula (19) for the scattering matrix, without any additional assumptions on geometrical or physical parameters of the network. Actually the analytical job of perturbation theory which is still present in (5) is reloaded by (19) on computing with finite matrices. Hence the formula (19) opens, in particular, a semi-analytic way of calculating of transmission coefficients across any junction.

Scattering matrix on the essential spectral interval.

- Comparison of the formula (19) with (5) implies the equation

$$\tilde{\mathcal{DN}}^{00}_{++} - \tilde{\mathcal{DN}}^{01}_{++} \frac{I}{\tilde{\mathcal{DN}}^{11}_{++} + K^1_+} \tilde{\mathcal{DN}}^{01}_{++} = \mathcal{DN}^F. \qquad (20)$$

Scattering matrix on the essential spectral interval.

- The terms of (20) contain sophisticated singularities inherited from the operator L_{int}. We are able to transform this expression to another form, with all singularities compensated. We observe first the compensation singularities in **DN**, representing it Krein's form. Denote

$$\mathcal{T}_+ = \sum_{\lambda_s \in \Delta} \varphi_s \rangle\langle P_+^0 \frac{\partial \varphi_s}{\partial n} + P_+^1 \frac{\partial \varphi_s}{\partial n},$$

$$\mathcal{T}_- = \sum_{\lambda_s \in \Delta} \varphi_s \rangle\langle P_-^1 \frac{\partial \varphi_s}{\partial n},$$

and consider the rational approximation of **DN**

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

Intrinsic large parameter and analytic perturbation procedure.

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

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

Intrinsic large parameter and analytic perturbation procedure.

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

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

$$\tilde{\mathbf{DN}} = \mathbf{DN}_{++} - \mathbf{DN}_{+-} \frac{I}{\mathcal{DN}^{11}_{--}(\Delta) + \mathcal{K}^{11}_{--} + K^{1}_{-}} \mathbf{DN}_{-+}. \quad (21)$$

Intrinsic large parameter and analytic perturbation procedure.

- Compensation of singularities in (21) inherited from the spectrum of L_{int} can be observed in the same way as the compensation of singularities in (6). Introduce

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

and

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

Intrinsic large parameter and analytic perturbation procedure.

- Introduce the notation:

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

Intrinsic large parameter and analytic perturbation procedure.

- **Theorem on compensation of singularities 2** *The Krein formula (21) for the* $\mathbf{\tilde{DN}}$ *can be re-written on the essential spectral interval, as:*

$$\mathbf{\tilde{DN}} = \mathbf{K}_F + \mathcal{J}T^+\rangle \frac{I}{\lambda I - L^\Delta + Q(\lambda)} \langle T\mathcal{J}^+. \qquad (22)$$

The representation (21) remains valid on a complex neighborhood G_Δ *of the essential spectral interval.*

Intrinsic large parameter and analytic perturbation procedure.

- Note that the expression (20) is the Schur complement of the matrix

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

  Absence of singularities at the spectrum of L_{int} in (22) is inherited by the Schur complement. Inserting the Schur complement into (19) gives an explicit formula for the scattering matrix of the junction in form.

Intrinsic large parameter and analytic perturbation procedure.

- $$S(\lambda) = \frac{iK_+ - \left[\mathcal{D}\mathcal{N}_\Delta^F + \mathcal{K}_\Delta^F\right]}{iK_+ + \left[\mathcal{D}\mathcal{N}_\Delta^F + \mathcal{K}_\Delta^F\right]}, \tag{23}$$

  with the denominator preceding the numerator. The details of this representation can be recovered, if needed, from the above theorem. Note that the above expression (23) for the scattering matrix can be simplified if some additional assumption is imposed on K_+, $\mathcal{K}_\Delta^F$.

Intrinsic large parameter and analytic perturbation procedure.

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

$$\sup_{\lambda\in\Delta} \| [K_+]^{-1}(\lambda), \mathcal{K}_\Delta^F(\lambda) \| < 1, \ \lambda \in \Delta.$$

Intrinsic large parameter and analytic perturbation procedure.

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

$$S_{ess}(\lambda) = \frac{iK_+ - \mathcal{DN}^F_\Delta}{iK_+ + \mathcal{DN}^F_\Delta}, \tag{24}$$

where the intermediate DN-map $\mathcal{DN}^F = \mathcal{DN}^F_\Delta + \mathcal{K}^F_\Delta$ is substituted by the essential polar part $\mathcal{DN}^F_\Delta$.

Intrinsic large parameter and analytic perturbation procedure.

- The essential scattering matrix can be interpreted as a scattering matrix of a solvable model of the junction, see [14]. The corresponding resonances - vector zeros $(\lambda_0, e_{\lambda_0})$ can be found from the algebraic equation

$$\left[iK_+ - \mathcal{D}\mathcal{N}_\Delta^F\right] e_0 = 0.$$

They define the speed of transition processes in the junction and the resonance character of thew transmission across the junction.

Intrinsic large parameter and analytic perturbation procedure.

- Due to operator version of Rouche theorem, [16], the zeros of the scattering matrix are close to zeroes of (24), which are found from an algebraic equation. The efficiency of the jump-start as the first step of the analytic perturbation procedure is defined by the precision of calculation of the zeros of the scattering matrix.

Jump-start in analytic perturbation procedure for scattering matrix.

- One can consider a perturbation $\mathcal{L} \longrightarrow \mathcal{L}_\varepsilon$ of the original scattering problem on quantum wires which reduces the transparency of the junction $\Omega = \Omega_{int} \cup \omega$. It may be, for instance, an erection of barriers hight ε^{-1} on the bottom sections Γ. Then the intermediate DN-map of the perturbed problem on the essential spectral interval will approach the DN-map of the Schrödinger operator L_{int} on the quantum well and the zeros $p_s^2(\varepsilon)$ of the scattering matrix will approach the the eigenvalues λ_s of L_{int}. The complex conjugate poles $\bar{p}_s^2(\varepsilon)$ of the scattering matrix will be approaching the eigenvalues λ_s of L_{int} too, hence the corresponding Blaschke- factor of the scattering matrix

$$\frac{p_s(\varepsilon) - p}{\bar{p}_s(\varepsilon) - p} \; P_s(\varepsilon) + [I - P_s(\varepsilon)] := B_s(\varepsilon, p).$$

Jump-start in analytic perturbation procedure for scattering matrix.

- This Blaschke-factor is not an analytic function of ε, p in a neighborhood of $0, \sqrt{\lambda_s}$. All other factors $B_t(\varepsilon, p),\ t \neq s$, which correspond to neighboring eigenvalues $\lambda_t \neq \lambda_s$, are analytic near $0, \sqrt{\lambda_s}$. Hence, the scattering matrix $S(\varepsilon, p)$ after eliminating the factor B_s

$$S_0^s(\varepsilon, p) = S(\varepsilon, p)\ \ [B_s(\varepsilon, p)]^{-1}$$

becomes an analytic function of (ε, p) near the point $\left(0, \sqrt{\lambda_s}\right)$.
The above elimination of the non-analytic actor of the scattering matrix may be done taking into account the time-reversal symmetry of the scattering matrix of the real Schrödinger operator $\mathcal{L}$ on the network $S(k) = S^+(-\bar{k})$.

Jump-start in analytic perturbation procedure for scattering matrix.

- Then, for given symmetric factor

$$B^{sym}(p,\varepsilon) = B(p,\varepsilon)\bar{B}(-p,\varepsilon) \tag{25}$$

of the scattering matrix, one can find an *intermediate operator* L^0_ε on a star-shaped quantum graph, such that

$$S(L^0_\varepsilon, I^\omega) = B^{sym}(p,\varepsilon)$$

and the remaining factor $S_0(\varepsilon,p) = S(\varepsilon,p)\ \left[B_s^{Sym}(\varepsilon,p)\right]^{-1}$ is, due to the chain-rule for scattering matrices, coincides with $S(\mathcal{L}_\varepsilon, L^0_\varepsilon)$:

$$I^\omega \xrightarrow{B^{sym}(p,\varepsilon)} L^0_\varepsilon \xrightarrow{S_0(\varepsilon,p)} S(\mathcal{L}_\varepsilon)$$

Jump-start in analytic perturbation procedure for scattering matrix.

- The intermediate operator L_ε^0 plays a role of the *jump-start* in analytic perturbation procedure, which deals with non-analytic first step. The second step of the procedure provides a geometrically convergent series.
  The semi-analytic method of calculation of the scattering matrix, based on the formula (19) allows to calculate the symmetric factor of the scattering matrix with a good precision, and construct the corresponding intermediate operator L_ε^0. Unfortunately even high degree of precision does not allow to find an exact expression for $B^{sym}(p, \varepsilon)$, such that the remaining part of the scattering matrix, after elimination of the constructed expression, is analytic with respect to ε near the origin.

Jump-start in analytic perturbation procedure for scattering matrix.

- Nevertheless our approach permits to suggest a solvable model of a thin junction in form of a quantum graph, see [14]. This confirms the hypothesis of H. Poincare,[17], concerning the role of resonances in analytic perturbation procedure. Our solvable model is automatically fitted- its scattering matrix serves an approximation for the scattering matrix of the original junction. Fitting of solvable models constructed in operator extensions, see [18-20], remains, generally, a serious problem.

Jump-start in analytic perturbation procedure.

- Notice that Prigogine, see [21], inspired by the idea H. Poincare [17] about the role of resonances in analytic perturbation procedure, attempted to construct an "intermediate operator"- a version of our jump-start- as a tool of analytic perturbation procedure on continuous spectrum. His attempt was not successful, because he imposed, in advance, too strong conditions on the object of his search. In particular, he assumed that the intermediate operator should be a function of the non-perturbed hamiltonian. Our jump-start is obtained based on local rational approximation of the corresponding DN-map, and it is a finite-dimensional perturbation of the non-perturbed Hamiltonian, with the same leading resonance on the essential spectral interval.

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