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A star-graph model via operator extension

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Abstract

One usually assumes that the Schrödinger operator on a thin quantum network ("fattened graph") can be simulated by the ordinary Schrödinger operator on the corresponding one-dimensional quantum graph. On the other hand, each quantum graph can be constructed of standard elements – star graphs. We prove that a thin star-shaped quantum network which consists of a compact domain and a few straight semi-infinite quantum wires, with a two-dimensional Schrödinger operator on it, can be simulated by the corresponding solvable model in form of a one-dimensional star graph: an outer space, with an ordinary Schrödinger operator on the leads, a resonance vertex supplied with an inner space and a finite matrix in it and an appropriate boundary condition connecting the inner and outer components of elements from the domain of the model. The model is (locally) quantitatively consistent: the scattering matrix of the model on a certain spectral interval serves an approximation of the scattering matrix of the network. The role of the constructed star-graph model as a "jump-start" in analytic perturbation procedure on continuous spectrum is discussed.

1. *Introduction*

Generally, a Schrödinger operator with non-constant coefficients or one in a non-standard domain rarely admits spectral analysis in explicit form. For qualitative analysis of quantum systems the Schrödinger operator often is substituted by a solvable model, constructed by the von Neumann operator extension technique, [**1**], see for instance [**2–4**] and an extended list of references in [**5**]. In particular, the substitution of the network by a proper one-dimensional graph, with special boundary conditions at the vertices, looks like a convenient tool for the qualitative analysis of the Schrödinger equation on the network, see for instance [**3–16**]. Unfortunately the estimation of the error caused by the substitution of the network by the corresponding graph is difficult. Shrinking of the "fattened graph" Ω_δ to the one-dimensional graph was studied in numerous papers, see for instance [**11**, **14**, **17**, **18**]. The authors considered a compact network Ω_δ constructed of the vertex domains Ω_{in}, with diameter proportional to δ^α, $0 < \alpha < 1$ and several finite leads, width $\omega^m\ \delta \to 0$ joining them with each other. In [**17**] they developed, based on [**19**, **20**], a variational technique for description of the asymptotic behavior of the discrete spectrum of the Schrödinger operator on the quantum network Ω_δ of various grades α of thinness. It appeared that the (discrete) spectrum of the Laplacian on the compact shrinking "fattened graph" Ω_δ tends to the spectrum of the Laplacian on the corresponding one-dimensional graph but with different boundary

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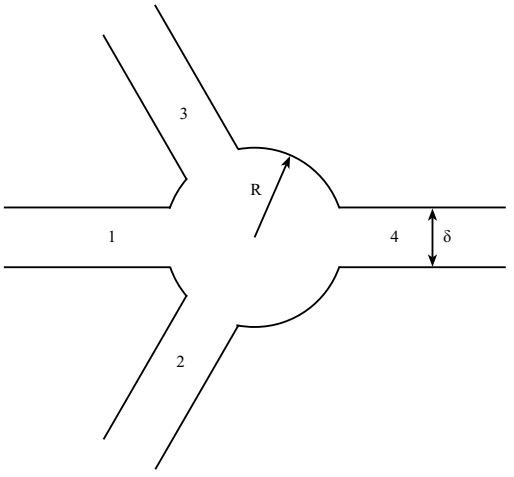


Fig. 1. Resonance triadic quantum switch.

conditions at vertices depending on the speed of shrinking: the Kirchhoff boundary conditions at the nodes, in the case of "small protrusion" $1/2 < \alpha < 1$ or the homogeneous Dirichlet boundary conditions, in case of " large protrusion", $0 < \alpha < 1/2$, see [**14**, theorems 1,2,3]. For recent results in this area see [**21**].

In this paper we consider thin quantum networks with small protrusion $\alpha = 1$, assuming diam $\delta \ll$ diam Ω_{in}. We will construct a *quantitatively consistent* solvable model of the quantum network, in the form of a star-graph with a vertex supplied with inner space and appropriate vertex Hamiltonian. The scattering matrix of the properly fitted model serves as a local approximation – on a certain "essential" spectral interval Δ – of the scattering matrix of the original network. In contrast to the quoted above results for compact networks, where the wave-functions are obtained based on a variational approach, we use Dirichlet-to-Neumann map $\mathcal{DN}^\Lambda$ of an intermediate Hamiltonian L_Λ, to derive an explicit formula for the scattered waves on the original network, see (5). The scattering matrix of the star-graph model is obtained via replacement of $\mathcal{DN}^\Lambda$ in (5) by the corresponding rational approximation on Δ. This defines all parameters of the model in terms of spectral characteristics of L_Λ. In course of construction and fitting of the solvable star-graph model we also define the energy-dependent boundary conditions at the vertex for the Schrödinger equation on the graph. In the simplest case when only one resonance eigenvalue λ_0 of the intermediate Hamiltonian is present on Δ, this condition depends linearly on the spectral parameter, and is parametrized by coordinates $\Re k_0$, $\Im k_0$ of the corresponding resonance.

Note that in [**9**] an algorithm for construction of the scattering matrix of the quantum graph of the scattering matrices of star-shaped elements is described and, in [**10**] a convenient formula for the scattering matrix of the star-graph in terms of the boundary parameters at the vertex is suggested. For extended discussion of properties of star graphs see [**22**, **23**].

2. *Scattering matrix via the intermediate Hamiltonian. The approximate scattering matrix*

The scattered waves of the Schrödinger operator $\mathcal{L}$ on the network, see for instance Figure 1 below, are obtained via matching, on the bottom sections of the wires, of the exponential solutions of the Schrödinger equation in the wires to the solutions of the equation on the quantum wells. Similar matching is usually done based on Dirichlet-to-Neumann

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map – a multi-dimensional analog of the Weyl-Titchmarsh function, see [**24–29**]. This gives an infinite system of linear equations for the scattered waves and scattering matrix, see in [**30**] numerous examples of calculation of the scattering matrices for simple domains, based on corresponding infinite linear systems. In [**32**] the Dirichlet-to-Neumann map of the intermediate Hamiltonian is used to obtain the scattering matrix as the solution of a *finite* linear system.

Scattering processes are observed in solids, for relatively low temperature, only on a small *essential spectral interval* Δ centered at the Fermi level, see [**31**]. This fact permits to develop the perturbation procedure for the one-body scattering problem on the network in two steps, substituting, on the first step, the original problem on the whole network by the corresponding solvable model, on the essential interval of the spectral parameter, and accomplishing, on the second step, by the standard analytic perturbation procedure for the perturbed problem, based on the solvable model. In this paper we construct the solvable model and fit it such that the model scattering matrix may serve a good local approximation for the complete scattering matrix on the essential spectral interval.

In this section, following [**32**] (see also [**33**] for more details) we introduce an intermediate Hamiltonian and give exact and approximate formulae for the scattering matrix in terms of the corresponding Dirichlet-to-Neumann map (DN-map) of the intermediate Hamiltonian. The role of the intermediate Hamiltonian is played by the first addendum of the Glazman's splitting $\mathcal{L}_\Lambda = L_\Lambda \oplus l_\Lambda$ of the original Schrödinger operator $\mathcal{L}$ on the whole network see [**34**]. The splitting is selected in dependence on the position of the Fermi level, scaled as $\Lambda = 2m_0\hbar^{-2}E_F$, see equations (1,2) below. The absolutely continuous spectra of both $\mathcal{L}$ and the split operator $\mathcal{L}_\Lambda = L_\Lambda \oplus l_\Lambda$ have the same band structure as the non-perturbed Schrödinger operator on the semi-infinite wires on the system $\omega = \bigcup_m \omega^m$ of all semi-infinite wires, with the constant potential $V^\omega = \{V^m\}$, and zero boundary condition on the boundary. Hereafter we use the scaled spectral parameter $\lambda = 2m_0\hbar^{-2}E$, the scaled effective masses $\mu = m\, m_0^{-1}$, $\mu^\parallel = m^\parallel m_0^{-1}$, $\mu^\perp = m^\parallel m_0^{-1}$ and scaled potentials on the wires. The spectral bands are defined (see [**35**]) by the thresholds found as eigenvalues of the Laplacian on the cross-sections of the wires. The channel spanned by the cross-section eigenfunction $\sin(\pi l y/\delta)$ is *closed* if the corresponding threshold exceeds the scaled Fermi-level: $\pi^2 l^2/2\,\mu^\perp\delta^2 + V^m > \Lambda$, and it is *open* if $\pi^2 l^2/2\,\mu^\perp\delta^2 + V^m < \Lambda$. The *maximal essential spectral band* is the spectral interval between the minimal threshold λ^Λ_{min} of the closed channel and the maximal threshold λ^Λ_{max} of the open channels. Without restriction of generality we may assume that the maximal essential spectral band is situated on the positive semi-axis, $[\lambda^\Lambda_{max}, \lambda^\Lambda_{min}] \subset [0, \infty)$. For any λ from the maximal essential spectral band the exponential modes

$$\exp\left(\pm\sqrt{2\mu^\parallel}\sqrt{\frac{\pi^2 l^2}{2\,\mu^\perp\delta^2} + V^m - \lambda}\,x\right)\sqrt{2/\delta}\sin\frac{\pi l y}{\delta} := e^{\pm i p_l^m x} e_l^m$$

of the homogeneous Schrödinger equation in the semi-infinite wires are decreasing or growing in closed channels, where $p_l^m = i|p_l^m|$, and oscillating in open channels where $p_l^m > 0$.

The spectral problem for the split operator is defined the following way, see [**32**, **33**]. Denote by U_Ω sufficiently smooth functions on the vertex domain Ω_{in} and by U^ω sufficiently smooth functions on the wires ω^m. Then the scaled Schrödinger equation on Ω_{in} and on ω^m

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can be written, with respect to local coordinates, in the form:

$$-\frac{1}{2\mu}\,\triangle\, U_{in} + V_{in}U_{in} = \lambda\, U_{in}$$

$$-\frac{1}{2\mu^{\|}}\frac{\partial^2 U^{\omega}}{\partial x^2} - \frac{1}{2\mu^{\perp}}\frac{\partial^2 U^{\omega}}{\partial y^2} + \mathbf{V}^{\omega}\, U^{\omega} = \lambda\, U^{\omega}, \tag{1}$$

with bounded measurable potential V_{Ω} on the well, and constant potentials $\mathbf{V}^{\omega} = \{V^m\}$ on the wires. We assume here that the scaled tensor of effective mass is isotropic on the quantum well Ω_{in}, but is anisotropic on the wires. By $\mu^{\|}$, $\mu^{\perp}$ we denote the diagonal matrices constituted by the corresponding components of the tensor of effective mass in the wires ω^m:

$$\mu^{\|} := \lceil \mu_m^{\|} \rfloor\,,\ \mu^{\perp} := \lceil \mu_m^{\perp} \rfloor.$$

This assumption permits to observe the role of effective masses as components of the small parameter in the corresponding perturbation problem. We assume that all wires have the same width δ.

We consider the scattering problem for the Schrödinger equations (1) in $L_2(\Omega)$ on the quantum network $\Omega_{in} \bigcup_m \omega^m := \Omega$, with zero boundary conditions at the boundary $\partial\Omega$ and matching conditions at the bottom sections γ^m of the wires $\gamma^m \subset \partial\Omega_{in}$.

Denote by e_l^m the normalized cross-section eigenfunctions $\sqrt{2/\delta}\sin \pi l y/\delta$ in the semi-infinite wires and by $e_l^m\rangle\langle e_l^m := P_l^m$ the corresponding ortho-projections in $L_2(\gamma^m)$ of square-integrable functions on the bottom sections. Form e_l^m we form the *entrance subspaces*

$$E_+ = \bigvee_{open} e_l^m,\ E_- = \bigvee_{closed} e_l^m,$$

of open and closed channels, with corresponding projections, respectively

$$P_{\pm} = \sum_{open,\, closed} \oplus P_l^m.$$

We define the partial matching of U_{Ω} and U^{ω} on Γ by the following boundary conditions, applied on the union $\Gamma = \bigcup_m \gamma^m$ of the wires:

$$P_+ U_{in}|_{\Gamma} = P_+ U^{\omega}|_{\Gamma} = 0,\ \ P_-[U_{in} - U^{\omega}]|_{\Gamma} = 0,\ \ P_-\left[\frac{1}{2\mu}\frac{\partial U_{in}}{\partial n} - \frac{1}{2\mu^{\|}}\frac{\partial U^{\omega}}{\partial n}\right]\Bigg|_{\Gamma} = 0. \tag{2}$$

The partial boundary conditions (2) are consistent for $U \in W_2^2(\Omega)$, if the wires are attached orthogonally to flat pieces of the boundary of the the quantum well, and the Meixner condition is imposed at the inner corners of $\partial\Omega$. Really, the boundary values u_{Γ} of the W_2^2-functions in Ω_{in}, ω^m and the corresponding boundary currents $(1/2\mu)(\partial u/\partial n|_{\gamma^m})$ on Γ belong to $W_2^{3/2}(\partial\Omega_{in})$, $W_2^{1/2}(\partial\Omega_{in})$ respectively and the cross-section eigenfunctions (cse) e_m^l can be continued by zero from γ^m onto $\partial\Omega_{int}$ as elements of $W_2^{3/2}(\partial\Omega_{in})$.

The split operator $\mathcal{L}_{\Lambda} = L_{\Lambda} \oplus l_{\Lambda}$ is presented as an orthogonal sum of two self-adjoint operators: the trivial part l_{Λ} in the open channels $E_+ \times L_2(0,\infty) := \mathcal{H}^F_{open}$ and the non-trivial part L_{Λ} in the orthogonal complement $L_2(\Omega) \ominus \mathcal{H}^F_{open} := \mathcal{H}^F$.

The non-trivial part L_{Λ} is a self-adjoint operator in $\mathcal{H}^F$. The absolutely-continuous component of the spectrum σ_{ac} coincides with the absolutely – continuous spectrum of the part

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of the unperturbed operator

$$L_{out}^{closed} = -\sum_{closed} \frac{1}{2\mu^{\|}} \frac{\partial^2 U^{\omega}}{\partial x^2} - \frac{1}{2\mu^{\perp}} \frac{\partial^2 U^{\omega}}{\partial y^2} + \mathbf{V}^{\omega} U^{\omega}$$

in closed channels $E_- \times L_2(0, \infty)$, with zero boundary conditions on Γ, and fills the interval $[\lambda_{min}, \infty)$ with varying multiplicity. We call L_Λ intermediate Hamiltonian. Consider the intermediate boundary problem with boundary condition

$$\begin{aligned} \mathcal{L}u = \lambda u, \Im\lambda \neq 0, u \in L_2(\omega), \\ u \perp \mathcal{H}_+^F,\ u\big|_\Gamma = u_\Gamma \in E_+. \end{aligned} \tag{3}$$

The solution of the boundary problem (3) exists and is unique. It can be presented in Ω_{in} via re-normalized simple-layer potential with the corresponding Poisson kernel

$$P^\Lambda(x, x', \lambda) = -\frac{1}{2\mu} \frac{\partial G^\Lambda(x, x', \lambda)}{\partial n_{x'}},\ x' \in \Gamma,\ x \in \Omega_{int},$$

obtained via differentiation of the kerned of the resolvent of the intermediate operator restricted onto Ω_{in}. Then

$$u(x) = \int_\Gamma P^\Lambda(x, x', \lambda) u_\Gamma(x') d\Gamma.$$

The corresponding boundary current on Γ in open channels is defined as:

$$P_+ \frac{1}{2\mu} \frac{\partial u}{\partial n}\bigg|_\Gamma = -\frac{1}{4\mu^2} \int_\Gamma \frac{\partial^2 G^\Lambda(x, x', \lambda)}{\partial n_x \partial n_{x'}} u_\Gamma(x') d\Gamma \coloneqq \mathcal{DN}^\Lambda u_\Gamma. \tag{4}$$

Thus, based on (4) we introduce the DN-map $\mathcal{DN}^\Lambda$ of the intermediate Hamiltonian and calculate the scattering matrix S in terms of $\mathcal{DN}^\Lambda$ matching the scattering Ansatz in open channels

$$\Psi(x, e) = e^{-iK_+x} e + e^{iK_+x} S e,\ e_+ \in E_+,$$

to the appropriate solution of the intermediate boundary problem:

$$u_\Gamma = \Psi(x, e)|_\Gamma,\ \frac{1}{2\mu} \frac{\partial u}{\partial n}\bigg|_\Gamma = \frac{1}{2\mu_{\|}} \frac{\partial \Psi}{\partial n}\bigg|_\Gamma.$$

We recover the scattering matrix from this equation requires solving only a finite linear system, see [**32**]:

$$\mathbf{S}(\lambda) = \frac{\mathcal{DN}^\Lambda(\lambda) + \frac{i}{2\mu^{\|}} K_+(\lambda)}{-\mathcal{DN}^\Lambda(\lambda) + \frac{i}{2\mu^{\|}} K_+(\lambda)}. \tag{5}$$

Here

$$K_+(\lambda) = \oplus \sum_{open} p_l^m(\lambda) P_l^m$$

is the exponent of the oscillating exponential modes $\exp[\pm i\ K_+ x\ ]\ e$ with $e \in E_+$, in the open channels. Similarly we introduce

$$K_-(\lambda) = \oplus \sum_{closed} |p_l^m(\lambda)| P_l^m, -$$

the exponent of decreasing modes $\exp\ [-K_- x\ ]\ e$ with $e \in E_-$, in the closed channels.

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We verified in [**32**], see also [**33**] that for "thin" networks $\mathcal{DN}^\Lambda$ in (5) can be replaced locally, with a minor error, on a certain essential spectral interval $\Delta \subset [\lambda^\Lambda_{max}, \lambda^\Lambda_{min}]$, by an appropriate rational approximation. We call this approximation an *essential DN map*- $\mathcal{DN}^\Lambda_\Delta(\lambda)$, and we define the corresponding essential scattering matrix on Δ as:

$$\mathbf{S}_\Delta(\lambda) = \frac{\mathcal{DN}^\Lambda_\Delta(\lambda) + \frac{i}{2\mu^\parallel}K_+(\lambda)}{-\mathcal{DN}^\Lambda_\Delta(\lambda) + \frac{i}{2\mu^\parallel}K_+(\lambda)}. \tag{6}$$

Here the essential DN map $\mathcal{DN}^\Lambda_\Delta(\lambda)$ contains only a finite number of poles at the eigenvalues of the intermediate Hamiltonian L_Λ on the essential spectral interval:

$$\mathcal{DN}^\Lambda_\Delta = \frac{1}{4\mu^2}\sum_{\lambda_r\in\Delta}\frac{\phi_r^+\rangle\,\langle\phi_r^+}{\lambda-\lambda_r}, \tag{7}$$

with $\phi_0^\pm = P_\pm(\partial\varphi_r/\partial n)|_\Gamma$. Note that the intermediate DN-map is connected with the classical DN – map $\mathcal{DN}$ defined via solution of the standard Dirichlet problem:

$$-\frac{1}{2\mu}\Delta u + V_{in}u = \lambda u,\ u|_{\partial\Omega_{in}\setminus\Gamma} = 0,\ u|_\Gamma = u_\Gamma :$$

$$\mathcal{DN}u_\Gamma \coloneqq \frac{1}{2\mu}\frac{\partial u}{\partial n}\bigg|_\Gamma. \tag{8}$$

To describe that connection we need to represent the classical DN-map as a matrix in the orthogonal decomposition of $L_2(\Gamma) \coloneqq E = E_+ \oplus E_-$:

$$\mathcal{DN} = \begin{pmatrix} P_+\mathcal{DN}P_+ & P_+\mathcal{DN}P_- \\ P_1\mathcal{DN}P_+ & P_-\mathcal{DN}P_- \end{pmatrix}.$$

In terms of the above matrix elements we have, see [**32**],

$$\mathcal{DN}^\Lambda = P_+\mathcal{DN}P_+ - P_+\mathcal{DN}P_-\mathbf{D}^{-1}P_-\mathcal{DN}P_+,$$

with

$$\mathbf{D} = P_-\mathcal{DN}P_- + \frac{1}{2\mu^\parallel}K_-.$$

If the Fermi level is situated in the middle of $[\lambda_{max}, \lambda_{min}]$, then the exponent of closed channels K_- can be estimated near the Fermi-level by $(1/\sqrt{2\mu^\parallel})\sqrt{(2l+1)\pi^2/2\delta^2\mu^\perp} \approx \delta^{-1}$. If there is a single simple resonance eigenvalue λ_0 of L_{in} on Δ, then this implies the estimation of the denominator $\mathcal{D}$ for *thin* networks, $\delta/\operatorname{diam}\Omega_{in} \ll 1$, near the resonance eigenvalue $\lambda_0 \approx \Lambda$ of L_{in}:

$$\begin{aligned}\mathbf{D} &= \frac{1}{4(\mu)^2}\frac{\phi_0^-\rangle\,\langle\phi_0^-}{\lambda-\lambda_0} + K_- + \mathcal{K}_- \\ &= \left[\frac{1}{4(\mu)^2}\frac{\phi_0^-\rangle\,\langle\phi_0^-}{\lambda-\lambda_0} + \frac{1}{2\mu^\parallel}K_-\right]\left([1+O\left(\frac{\delta}{\operatorname{diam}\Omega_{in}}\right)\right],\end{aligned}$$

where ϕ_0 is the boundary current of the resonance eigenfunction Ψ_0 of Λ_{in}. This implies, see [**32**, **33**], existence of the resonance eigenvalue λ_0^Λ of the intermediate Hamiltonian near λ_0 and estimation for the corresponding boundary current

$$\lambda_0^\Lambda = \lambda_0 + 0(\delta/\operatorname{diam}\Omega_{in}),\ P_-\phi_0^\Lambda \approx P_-\phi_0,$$

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for thin networks. In particular, the substitution

$$\mathcal{DN}_{appr} := \frac{1}{4(\mu)^2} \frac{\phi_0^+\rangle\,\langle\phi_0^+}{\lambda - \lambda_0}$$

into the above expression (5) for the scattering matrix gives another convenient approximation for it in terms of spectral data of L_{in}

$$S_{appr}(\lambda) = \frac{\frac{1}{4(\mu)^2} \frac{\phi_0^+\rangle\,\langle\phi_0^+}{\lambda-\lambda_0} + \frac{i}{2\mu} K_+}{-\frac{1}{4(\mu)^2} \frac{\phi_0^+\rangle\,\langle\phi_0^+}{\lambda-\lambda_0} + \frac{i}{2\mu} K_+}. \tag{9}$$

One can attempt to connect directly the formula (5),(6) or (9) with a differential equation on wires, replacing the Schrödinger operator on Ω_{in} by an energy-dependent boundary condition at the union of bottom sections Γ. This trivialization, see section 6, although it permits us to calculate the exterior part of the scattered waves, does not respect important quantum – mechanical requirements: existence of the self-adjoint Hamiltonian, with a complete orthogonal system of eigenfunctions.

In this paper we will interpret the *few-pole approximation* (6) as a scattering matrix of a solvable Hamiltonian which satisfies the basic requirements of quantum mechanics. Our model is "structure-preserving" in a sense of [**36**]. In Section 3 we will construct the star-graph model of the quantum network of a single vertex, supplied with a Hamiltonian of the inner degrees of freedom, and several one-dimensional semi-infinite quantum wires emulating open channels in semi-infinite wires. In Section 4 we suggest the procedure of fitting of the solvable model. In Section 5 we will show that the model can be used as a jump-start in an analytic perturbation procedure. In Section 6 we discuss the energy-dependent boundary conditions at the nodes of the star-graph.

3. *Solvable model of the network via symplectic operator extension procedure*

The star-graph solvable model of the network will be constructed as a finite-dimensional perturbation of the orthogonal sum of the non-perturbed Hamiltonian l_Λ in the open channels and a finite matrix A acting in the *inner space* of the node. We will choose the parameters of the model such that the model scattering matrix coincides with the few-pole approximation $\mathbf{S}_\Delta$ of the complete scattering matrix $\mathbf{S}$. Then the constructed model will be automatically *quantitatively consistent*. The scattering Ansatz of the model in open channels satisfies on the maximal essential spectral band $[\lambda_{max}, \lambda_{min}]$ the same equation as the scattering Ansatz on the original network:

$$-\frac{1}{2\mu^{\|}} \frac{d^2U^\omega}{dx^2} + \sum_{s,m} \frac{\pi^2 s^2}{2\mu^\perp \delta_m^2} p_s^m U + \mathbf{V}^\omega U^\omega := l^\Lambda U^\omega = \lambda\, U^\omega,\ \lambda \in \Delta. \tag{10}$$

But the construction of the vertex part of the model will be done with a major change of the original intermediate operator.

Without restriction of generality we can assume that the essential spectral band Δ lies strictly inside of the maximal essential spectral band $\Delta \subset [\lambda^\Lambda_{max}, \lambda^\Lambda_{min}] \subset [0, \infty)$, and hence does not overlap with the continuous spectrum of the intermediate Hamiltonian L_Λ. This assumption is true for thin networks. According to [**33**] only a finite number N of eigenvalues of the intermediate operator are situated on Δ. Then substitution of (5) by (6) may cause, according to [**33**], only a minor and controllable error. Now we will prove that there exist a finite-dimensional perturbation of the operator $l_\Lambda \oplus A$ such that the scattering

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matrix of the perturbed operator coincides with $\mathbf{S}_\Delta$. The perturbation will be constructed via operator restriction-extension procedure applied to the orthogonal sum $l_\Lambda \oplus A$, where A is an $N \times N$ Hermitian matrix : $E_A \to E_A$, dim $E_A = N$. The parameters of the model will be properly selected to fit the spectral data of the intermediate Hamiltonian on the original quantum network, within the essential spectral interval Δ.

Assume that the positive matrix A is defined by its 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 β of the model, see below (19), will be defined later, based on comparison of the scattering matrix of the model with the essential scattering matrix (6).

Consider restrictions of both l_Λ and A to symmetric operators on the corresponding domains. The restriction of $l_\Lambda|_{D_0^l} = l_0$ is defined on functions vanishing near $x = 0$. Then the adjoint operator l_0^+ is defined on $W_2^2(E_+,\ R_+)$, and the boundary form of it is calculated via integration by parts:

$$\mathcal{J}_l(U,\ V) = \langle l_0^+ U,\ V\rangle - \langle U,\ l_0^+ V\rangle = \frac{1}{2\mu^\parallel}\langle U'(0),\ V(0)\rangle - \frac{1}{2\mu^\parallel}\langle U(0),\ V'(0)\rangle, \qquad (11)$$

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

Restriction of the matrix A is equivalent to selection of the deficiency subspace for the given value i of the spectral parameter. Choose a generating subspace N_i, $\overline{\bigvee_{k>0} A^k N_{-i}} = E_A$ such that $(A + iI)/(A - iI)N_i \bigcap N_i = 0$, 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 $A \to A_0 = A|_{D_0^A}$. We develop the extension procedure for general N_i and fit it later based on spectral data of the intermediate operator, see Theorem 4·1, 4·2. In our construction $N_i \subset E_A$ will play a role of the deficiency subspace at the spectral point i, dim $N_i = d,\ 2d \leqslant N$ and the dual deficiency subspace is $N_{-i} = (A + iI)/(A - iI)N_i$. 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 [**38**]. In this case the "formal adjoint" operator for A_0 is defined on the defect $N_i + N_{-i} \coloneqq \mathcal{N}$ by the von Neumann formula. $A_0^+ e \pm i\,e = 0$ for $e \in N_{\pm i}$. Then the extension is constructed, see Lemmas 3·1–3·4 below, via restriction of the formal adjoint onto a certain plane in the defect where the boundary form vanishes (a "Lagrangian plane"). According to the classical von Neumann construction all Lagrangian planes are parametrized by isometries $V : N_i \to N_i$ in 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 [**37**] there exist a self-adjoint extension A_V of the restricted operator A_0. We construct this extension based on the following.

LEMMA 3·1. *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.*

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Proof. Indeed, if A_V is the extension, then on the $\mathcal{T}_V$ 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 assumption of non-overlapping, see [**37**]. In particular, in the case $\dim E_A = 1$, which is not formally covered by the above procedure, was analyzed in [**39**] independently of [**37**]. The relevant formulae for the scattering matrix and scattered waves remain true and may be verified by the direct calculation. We will use this fact in Section 4.

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

$$u = \sum_{s=1}^{d} [x_s\, f_s + \hat{x}_s\, \hat{f}_s] \in \mathcal{N}, \tag{12}$$

by the von Neumann formula, see [**34**],

$$A_0^+ u = \sum_{s=1}^{d} [-i\ x_s\, f_s + i\ \hat{x}_s\, \hat{f}_s]. \tag{13}$$

In order to use the symplectic version of the operator-extension techniques we 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:

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

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

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

$$u = \sum_{s=1}^{d} [\xi_s^+\, w_{s,+} + \xi_s^-\, w_{s,-}]. \tag{14}$$

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

$$u = \frac{A}{A - iI} \vec{\xi}_+^{\,u} - \frac{1}{A - iI} \vec{\xi}_-^{\,u},\ \ A_0^+ u = -\frac{1}{A - iI} \vec{\xi}_+^{\,u} - \frac{A}{A - iI} \vec{\xi}_-^{\,u}. \tag{15}$$

The following formula of integration by parts for abstract operators was proved in [**38**]:

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LEMMA 3·2. *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

$$\mathcal{J}_A(u, v) = \langle A_0^+ u, v\rangle - \langle u, A_0^+ v\rangle = \langle \vec{\xi}_+^u, \vec{\xi}_-^v\rangle_N - \langle \vec{\xi}_-^u, \vec{\xi}_+^v\rangle_N. \tag{16}$$

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 $\{U'(0),\ U(0),\ V'(0),\ V(0)\}$. We will call them *symplectic coordinates* of the element u, v. The next statement proved in [**38**] is the core detail of the fundamental Krein formula [**40**], for generalized resolvents of symmetric operators. In our situation, it is used in course of calculation of the scattering matrix.

LEMMA 3·3. *The vector-valued function of the spectral parameter*

$$u(\lambda) = \frac{A + iI}{A - \lambda I}\ \ \vec{\xi}_+^u := u_0 + \frac{A}{A - iI}\vec{\xi}_+^u - \frac{1}{A - iI}\vec{\xi}_-^u, \tag{17}$$

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

$$\vec{\xi}_-^u = -P_{N_i}\frac{I + \lambda A}{A - \lambda}\vec{\xi}_+^u. \tag{18}$$

Introduce the function

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

It has a positive imaginary part in the upper half-plane $\Im\lambda > 0$ and serves an abstract analog of the celebrated Weyl–Titchmarsh function. The operator-function $\mathcal{M}$ exists almost everywhere on the real axis λ, and has a finite number of simple poles at the eigenvalues α_r^2 of A. This function plays an important role in description of spectral properties of self-adjoint extensions of symmetric operators, see [**40**, **42**].

We construct a solvable model of the quantum network as a self-adjoint extension of the orthogonal sum $l_0 \oplus A_0$. We consider 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 corresponding elements in the deficiency subspaces. For instance, one may select a finite-dimensional operator $\beta: E_+ \oplus N_i \to E_+ \oplus N_i$ and define the Lagrangian plane $\mathbf{L}_\beta$ by the boundary condition

$$\begin{pmatrix} \frac{1}{2\mu^\parallel}U'(0) \\ -\vec{\xi}_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta_{01}^+ & 0 \end{pmatrix}\begin{pmatrix} U(0) \\ -\vec{\xi}_- \end{pmatrix}. \tag{19}$$

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The extension defined by (19) 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 [**37**]. 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 (19). 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_Λ of the split operator $\mathcal{L}_\Lambda$ (in the open channels). The corresponding eigenfunctions of $\mathbf{A}_\beta$ on the maximal essential spectral band $[\lambda^\Lambda_{\max},\ \lambda^\Lambda_{min}] \supset \Lambda$ can be found, see [**5**], via substitution into the above boundary condition for the column, combined of the scattering Ansatz in open channels with (17) and in the outer space:

$$\Psi = \begin{pmatrix} e^{-iK_+x}\nu + e^{iK_+x}\mathbf{S}\nu \\ \frac{A+iI}{A-\lambda I}\vec{\xi}^{\,u}_+ \end{pmatrix}. \tag{20}$$

It gives the linear equation for scattering matrix:

$$\begin{pmatrix} -\frac{i}{2\mu^\parallel}K_+(\nu - S\nu) \\ -\vec{\xi}_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta^+_{00} & 0 \end{pmatrix} \begin{pmatrix} \nu + S\nu \\ \mathcal{M}\vec{\xi}_+ \end{pmatrix}.$$

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

LEMMA 3·4. *The scattering matrix for the constructed extension is an analytic function of the spectral parameter* λ:

$$\mathbf{S}(\lambda) = \frac{\frac{i}{2\mu^\parallel}K_+ + [\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}]}{\frac{i}{2\mu^\parallel}K_+ - [\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}]}, \tag{21}$$

with the denominator of the fraction preceding the numerator. The coordinate $\vec{\xi}_+$ *of the inner component of the scattered wave* (20) *is defined as* $\vec{\xi}_+ = -\beta^+_0(I + \mathbf{S})\nu$.

4. *Fitting of the solvable model*

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

$$Q_s = P_i P_s P_i.$$

Then the above expression takes the form :

$$[\beta_{00} - \beta_{01}\mathcal{M}\beta_{10}] = \left[\beta_{00} + \sum_{r=1}^{N_T} \alpha_r^2 \beta_{01} Q_{sr} \beta_{10}\right] + \sum_r^{N_T} \frac{1+\alpha_r^4}{\alpha_r^2 - \lambda}\beta_{01}Q_r\beta_{10}. \tag{22}$$

We will define the boundary parameters $\beta_{10},\ \beta_{01} = \beta^+_{10}$ later, but once they are defined, we choose β_{00} such that the first summand in the right-hand side of (22) vanishes: $\beta_{00} + \sum_r \alpha_r^2 \beta_{01} Q_r \beta_{10} = 0$. Then the scattering matrix takes the form:

$$\mathbf{S}(k) = \frac{\frac{i}{2\mu^\parallel}K_+ - \sum_{r=1}^{N_T} \frac{1+\alpha_r^4}{\alpha_r^2-\lambda}\beta_{01}Q_r\beta_{10}}{\frac{i}{2\mu^\parallel}K_+ + \sum_{r=1}^{N_T} \frac{1+\alpha_r^4}{\alpha_r^2-\lambda}\beta_{01}Q_r\beta_{10}}, \tag{23}$$

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

$$\sum_{r=1}^{N_T} \frac{1+\alpha_r^4}{\alpha_r^2-\lambda}\beta_{01}Q_r\beta_{10} \tag{24}$$

coincides with the essential part $\mathcal{DN}_\Delta^\Lambda$ of the DN-map of the intermediate operator – the finite sum of pole terms

$$\sum_{r=1}^{N_T} \frac{P_+\frac{1}{2\mu}\frac{\partial\varphi_r}{\partial n}\rangle\langle P_+\frac{1}{2\mu}\frac{\partial\varphi_r}{\partial n}}{\lambda_r-\lambda}. \tag{25}$$

Summarizing these results we obtain the following conditional statement for the extension constructed based on the boundary condition (19) in case when $N_i \bigcap N_{-i} = 0$ or dim $E_A = 1$:

THEOREM 4·1. *The constructed operator $\mathbf{A}_\beta$ is a solvable model of the Quantum network on the essential interval Δ, if and only if the dimension of the space E_A coincides with the number N_T of eigenvalues of the intermediate operator on $\Delta \subset [\lambda_{max}, \lambda_{min}]$, the eigenvalues α_r^2 of the inner Hamiltonian $A = \sum_{r=1}^{N_T}\alpha_r^2\nu_r\rangle\langle\nu_r$ coincide with eigenvalues of the intermediate operator on Δ, there exists a deficiency subspace N_i of the inner Hamiltonian such that $N_i \bigcap \frac{A+iI}{A-iI}N_i = 0$ and the operator $\beta_{01}: N_i \to E_+$ such that for the ortho-normal basis $\{e_s\}_{s=1}^{N_T}$ of eigenvectors of A in E_A*

$$P_+\frac{1}{2\mu}\frac{\partial\varphi_r}{\partial n} = \left[1+\alpha_r^4\right]^{1/2}\beta_{01}P_{N_i}\nu_r,\ r=1,2,\dots,N_T. \tag{26}$$

Eliminating the inner variables, we can reduce the model to the Schrödinger equation with the constant potential on open channels, and appropriate boundary conditions on the bottom sections:

$$\frac{1}{2\mu^\parallel}\frac{dU^\omega}{dx}\bigg|_\Gamma = \sum_{r=1}^{N_T}\frac{P_+\frac{1}{2\mu}\frac{\partial\varphi_r}{\partial n}\rangle\langle P_+\frac{1}{2\mu}\frac{\partial\varphi_r}{\partial n}}{\lambda_r-\lambda}U^\omega\bigg|_\Gamma. \tag{27}$$

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

Dr. M. Harmer suggested an important strengthening of the previous conditional statement, by proving a general theorem of existence of the subspace N_i and the projection P_{N_i} which satisfy the condition of Theorem 4·1. The proof we provide below only slightly differs from the original proof in [**44**]: we added the explicit formulae for β_{01}, P_{N_i} in terms of the corresponding Gram matrix.

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

$$\sum_s [1+\alpha_s^4]^{-1/2}P_+\frac{1}{2\mu}\frac{\partial\varphi_s}{\partial n}\bigg|_\Gamma\langle *,\varphi_s\rangle := \Phi_\Delta \tag{28}$$

from E_Δ to E_+,dim $E_+ = \mathbf{n}$.

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THEOREM 4·2 (M. Harmer). *The map Φ_Δ defines a one-to-one correspondence between 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_Δ is a generating subspace of L_Λ^Δ and

$$N_\Delta \bigcap \left(L_\Lambda^\Delta - iI\right)^{-1} \left(L_\Lambda^\Delta + iI\right) N_\Delta = 0, \tag{29}$$

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

Remark. This theorem gives an interpretation of the solvable model described in Theorem 4·1, in terms of the intermediate Hamiltonian via selection of the inner Hamiltonian A as a part L_Λ^Δ of L_Λ in the invariant subspace corresponding to the essential spectral interval Δ. The subspace $N_\Delta \subset E_\Delta$ plays the role of the deficiency subspace N_i of the inner Hamiltonian and $(L_\Lambda^\Delta - iI)^{-1}(L_\Lambda^\Delta + iI)N_\Delta$ plays the role of the dual subspace N_{-i}.

Proof. The map Φ_Δ is represented by the $\mathbf{n} \times N_T$ matrix Φ of columns ϕ_s with respect to the orthogonal basis of cse-functions $\{e_t\}$ in E_+. The condition (26) is equivalent to the representation of the operator Φ_Δ in form $\beta_{01}\ P_{N_i}$, where β_{01} is a bounded operator acting from E_A into E_+ and P_{N_i} is an orthogonal projection in E_A onto the deficiency subspace N_i. We will construct both $\beta_{01},\ P_{N_i}$ from the data encoded in Φ.

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

$$\Phi\ \Phi^+ = U^+ D\ \ U.$$

The non-negative diagonal matrix D is invertible on the orthogonal complement $\hat{E}$ of the corresponding null-space $\hat{E}_0$. We denote the restriction D onto $\hat{E}$ by $\hat{D}$. One can assume that the subspace $\hat{E}$ belongs to some extended space $\hat{E} \oplus \hat{E}_0$ which contains E_A, and the operator U^+ acts from $\hat{E} \oplus \hat{E}_0$ onto E_+ as an isometry. The operator $U^+ \hat{D}^{1/2}$ coincides with Φ. Hence the operator Φ is presented as a product $\beta \hat{P}$, with $\beta = \beta_{01} = U^+ \hat{D}^{1/2}: \hat{E} \to E_+$ and $\hat{P} = P_{\hat{E}} := P_{N_i} \subset E_A$, $\dim N_i = \dim \hat{E} = d$ and coincides with the dimension of the resonance entrance subspace of the intermediate operator. Up to some non-essential isometry we may assume that $E_A = E_\Delta, A = L_\Lambda^\Delta,\ N_i = N_\Delta$. The condition (29) guarantees that $N_i \bigcup N_{-i} = 0$.

In case when only one resonance eigenvalue α_0^2 of the intermediate operator sits on the essential spectral band, the obtained model scattering matrix

$$\mathbf{S}(p) = \frac{\frac{i}{2\mu^{\shortparallel}} K_+ - \frac{1+\alpha_0^4}{\alpha_0^2 - \lambda} \beta_{01} Q_0 \beta_{10}}{\frac{i}{2\mu^{\shortparallel}} K_+ + \frac{1+\alpha_0^4}{\alpha_0^2 - \lambda} \beta_{01} Q_0 \beta_{10}} \tag{30}$$

is a single-pole approximation of the scattering matrix of the network. The condition of the above theorem is obviously fulfilled for the single-pole approximation, when $P_+(\partial\varphi_0/\partial n) \neq 0$, $d = 1$, $N = 1$, and β_0 is a one-dimensional operator mapping the one-dimensional subspace N_i onto the resonance entrance subspace in E_+ spanned by $P_+(\partial\varphi_0/\partial n)$. For thin or shrinking networks one can estimate, (see [**32**] and more detail in [**33**]) the deviation of the single-pole and/or few-poles approximations from the exact scattering matrix on the network, in terms of the ratio $d/\operatorname{diam} \Omega_{in}$.

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We postpone the discussion of the non-stationary scattering matrix for QN to forthcoming publications. But we notice here that the local wave operators (see [**45**]) and the corresponding scattering matrix on the essential spectral band can be defined for the pair $(\mathcal{L}, \mathbf{A}_\beta)$.

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

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

Consider a thin quantum network constructed of a quantum well Ω_{in} and a single quantum wire of width δ attached to it, $\delta/\operatorname{diam}\Omega_{in} \ll 1$. Assume that the Fermi level is situated on the first spectral band in the wire, which has multiplicity 1. Without loss of generality we may assume that the component of the corresponding solvable model in the open channel is presented by the Schrödinger equation with $2\mu^{\|} = I$, $V^\omega = V$, $K_+ = p = \sqrt{\lambda - \frac{\pi^2}{2\mu^\perp \delta^2} - V}$ and one-dimensional subspace E_+:

$$-u'' = p^2 u, \ 0 < x < \infty. \tag{31}$$

Assume that the model Hamiltonian $\mathbf{A}_\beta$ is constructed as suggested in the previous section based on the "inner Hamiltonian" A, the differential operator l_Λ and the boundary parameters which are reduced to the coupling constant $\beta_{01} \coloneqq \beta$. Hereafter we will use the re-normalized eigenvalues $\alpha_s^2 - \pi^2/2\mu^\perp\delta^2 - V \coloneqq k_s^2 > 0$. Introducing that notation into the Krein function, and submitting the boundary parameter to the condition $\beta_{00} + \sum_{s=1}^N \alpha_s^2 \beta_{01} q_s \beta_{10} = 0$ we obtain the corresponding few-pole scattering matrix as a function of the wave-number p, with physically meaningful limit behavior at infinity $\mathbf{S}^\beta(p) \to I$:

$$\mathbf{S}^\beta(p) = \frac{ip - \beta^2 \sum_s \frac{1+\alpha_s^4}{k_s^2 - p^2} q_s}{ip + \beta^2 \sum_s \frac{1+\alpha_s^4}{k_s^2 - p^2} q_s}. \tag{32}$$

Here $q_s = |\langle e, e_s\rangle|^2$. Zeros $p_s(\beta)$ of the Scattering matrix (32) – the resonances – sit in the upper half-plane $\Im p > 0$ and approach the points $\pm k_s$, $k_{-s} \coloneqq -k_s$, when $\beta \to 0$.

Assume that the resonance eigenvalue $\alpha_0^2 = k_0^2 + (2\mu^\perp)^{-1}\delta^{-2}\pi^2 + V$ is situated close to the scaled Fermi-level Λ and the coupling constant $\beta \coloneqq \beta_{01}$ is relatively small, see below. Separating the resonance term in the numerator and denominator of (32)

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

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

$$p = k_0 - \frac{\beta^2\big(1+\alpha_0^4\big)q_0}{(p+k_0)\left(ip - \beta^2 \sum_{s\neq 0} \frac{1+\alpha_s^4}{k_s^2 - p^2} q_s\right)}. \tag{33}$$

Another resonance originated from the point $-k_0$ corresponds to the same eigenvalue, and it sits at the symmetric point $-\bar{k}_0(\beta)$ with respect to the imaginary axis. Remaining resonances $k_s(\beta)$, $s \neq 0$, can be found from similar equations. All functions $k_s(\beta)$ are analytic

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functions of β, k in small neighborhoods of $(0, \pm k_s)$. They sit in the upper half-plane symmetrically with respect to the imaginary axis $k_{-s}(\beta) = -\bar{k}_s(\beta)$. The scattering matrix (32) is unitary on the real axis k and has poles at the complex-conjugate points $\bar{k}_s(\beta)$ in the lower half-plane, and hence it is presented by the finite Blaschke product which tends to 1 when $|k| \to \infty$:

$$\mathbf{S}^\beta(p) = \prod_s \frac{p - k_s(\beta)}{p - \bar{k}_s(\beta)}. \tag{34}$$

The outer component of the scattered wave is presented as

$$u_0^\beta = e^{-ipx} + \mathbf{S}^\beta(k) e^{ipx}.$$

It fulfills appropriate boundary condition at the place of contact with the model quantum dot. The inner component of the scattered wave can be obtained from Lemma 3·4.

We explore the model scattering problem for small values of β. Though the resonances depend analytically on β, neither the scattering matrix (32,34) nor the scattered wave depend analytically of (β, p) on the product of a small neighbourhood of the origin in β-plane and small neighbourhoods of $\pm k_0$ in p-plane. The analyticity is lost due to presence of the points $\pm k_0$ where the resonances are created at $\beta = 0$: both $k_0(\beta)$ and $\bar{k}_0(\beta)$ approach the same point k_0 when $\beta \to 0$. The corresponding "resonance" factor of the scattering matrix

$$\mathbf{S}_0^\beta(p) = \frac{[p - k_0(\beta)]\,[p + \bar{k}_0(\beta)]}{[p - \bar{k}_0(\beta)]\,[p + k_0(\beta)]}. \tag{35}$$

is non-analytic on $(\Omega_\beta \times \Omega_{k_0} \times \Omega_{-k_0})$, though $k_\beta = \Re k_\beta + i\Im k_\beta$ is analytic function of β due to (33). But the complementary factor of the scattering matrix

$$\mathbf{S}_\beta^0(p) = \prod_{s \neq 0} \frac{p - k_s(\beta)}{p - \bar{k}_s(\beta)}, \tag{36}$$

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

THEOREM 5·1. *There exists a one-dimensional perturbation $\mathbf{A}_0^\beta$ of the operator*

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

with a non-trivial inner component, such that the scattering matrix of the pair $(\mathbf{A}_0^\beta, l_0)$ coincides with $-\mathbf{S}_0^\beta(p)$. Then the scattering matrix $\mathbf{S}$ of the complementary pair $(\mathbf{A}_\beta, \mathbf{A}_0^\beta)$ is equal to the complementary factor $-\mathbf{S}_\beta^0(p)$:

$$\mathbf{S}^\beta(p) = \mathbf{S}_0^\beta(p)\ \mathbf{S}_\beta^0(p).$$

The complementary factor is an analytic function of (β, k) on the product $(\Omega_\beta \times \Omega_{k_0} \times \Omega_{-k_0})$ of a small neighbourhood of the origin in β-plane and a small neighbourhood of the pair $(k_0, -k_0)$ 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 $\mathcal{M} = (1 + \alpha^2 \lambda)/(\alpha^2 - \lambda)$. 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 2×2

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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_+:

$$\begin{pmatrix} \Psi' \\ -\xi_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta_{10} & \beta_{11} \end{pmatrix} \begin{pmatrix} \Psi \\ -\xi_- \end{pmatrix}. \tag{37}$$

Substituting into the above equation the corresponding Ansatz for the wave-function of the problem (31) in the outer space

$$\Psi_0^\beta(x,\ p) = e^{-ipx} + \mathbf{S}^\beta(p)e^{ipx}, \tag{38}$$

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

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

Select the parameter β_{11} such that $1-\beta_{11}\alpha^2 = 0$, then $1+\beta_{11}\mathcal{M} = (\beta_{11}+\alpha^2)(\alpha^2-\lambda)$, and the scattering matrix with $\lambda = p^2 + \pi^2/2\mu^\perp\delta^2 + V$ takes the form:

$$\mathbf{S}_\beta(p) = -\frac{ip + \left[\beta_{00} - \frac{|\beta_{01}|^2}{\alpha^2+\beta_{11}}\left(1 + \frac{\alpha^2\pi^2}{2\mu^\perp\delta^2} + \alpha^2 V\right)\right] - \frac{|\beta_{01}|^2}{\alpha^2+\beta_{11}}\alpha^2p^2}{-ip + \left[\beta_{00} - \frac{|\beta_{01}|^2}{\alpha^2+\beta_{11}}\left(1 + \frac{\alpha^2\pi^2}{2\mu^\perp\delta^2} + \alpha^2 V\right)\right] - \frac{|\beta_{01}|^2}{\alpha^2+\beta_{11}}\alpha^2p^2}, \tag{39}$$

which is compatible with the Blaschke product (35). Comparing (39) with (35)

$$-\mathbf{S}_0^\beta(p) = -\frac{[(p-k_0(\beta)]\,[p+\bar{k}_0(\beta)]}{[p-\bar{k}_0(\beta)]\,[p+k_0(\beta)]} = \frac{-p^2 + 2i\Im k_0(\beta)p + |k_0(\beta)|^2}{p^2 + 2i\Im k_0(\beta)p - |k_0(\beta)|^2} = \mathbf{S}_\beta(p),$$

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

$$\frac{\beta_{00} - \frac{|\beta_{01}|^2}{\alpha^2+\beta_{11}}\left(1 + \frac{\alpha^2\pi^2}{2\mu^\perp\delta^2} + \alpha^2 V\right)}{|k_0(\beta)|^2} = \frac{1}{2\Im k_0(\beta)} = \frac{|\beta_{01}|^2}{\alpha^2+\beta_{11}}\alpha^2. \tag{40}$$

The solution of this system is not unique, but it can be parametrized by β_{00}. If we choose, for instance

$$\beta_{00} = \frac{|k_0(\beta)|^2 + \frac{\pi^2}{2\mu^\perp\delta^2} + V}{2\Im k_0(\beta)},$$

then we obtain

$$\alpha^2 = \left(|k_0(\beta)|^2 + \frac{\pi^2}{2\mu^\perp\delta^2} + V\right)^{-1}$$

and

$$|\beta_{01}|^2 = \frac{\alpha^2 + \alpha^{-2}}{2\Im k_0(\beta)\,\alpha^2},$$

together with $\beta_{11} = \alpha^2$ this gives complete list of parameters of the model, up to the freedom in choosing $\arg\beta_{01}$.

COROLLARY 5·1. *The exterior component of the scattered wave of the operator* $\mathbf{A}_0^\beta$ *presented by the Ansatz* (38) *is not analytic with respect to the coupling constant* $\beta_{01} \coloneqq \beta$ *near the origin. The non-analyticity of the scattered wave is caused by the presence of the*

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non-analytic factor $-\mathbf{S}_0^\beta$ *in the Scattering matrix* $\mathbf{S}_0$. *From Theorem 4·1, we interpret this factor as the scattering matrix for the pair* $(\mathbf{A}_0^\beta,\ l_0)$. *The complementary factor* $-\mathbf{S}_\beta^0$ *is analytic with respect to the coupling constant* β. *It can be interpreted as the scattering matrix for the pair* $(\mathbf{A}^\beta, \mathbf{A}_0^\beta)$. *Summarizing our observation we suggest, for our example, the following two-steps modification of the analytic perturbation procedure on continuous spectrum*:

(a) *First step is the construction of the solvable model and calculation of the corresponding (non-analytic with respect to the coupling constant* β *at the origin) scattering matrix. This is "the jump-start" of the analytic perturbation procedure.*

(b) *Second step is the calculation of the analytic factor of the scattering matrix of the model by the standard analytic perturbation procedure. The analytic factor is interpreted as the scattering matrix between the constructed solvable model and the perturbed operator* $\mathbf{A}^\beta$.

The obtained connection between resonances and analytic perturbation series on the continuous spectrum recalls the connection between small denominators in celestial mechanics and divergence of perturbation series, observed by Poincaré, see [**48**]. *More historical comments about intermediate Hamiltonian and the jump-start may be found in* [**43**], *where similar modification of the analytic perturbation procedure for the Friedrichs model is suggested.*

Remark. Note that recovering *exact* information on the resonance $k_0(\beta)$ and on the corresponding residue for the perturbed operator $\mathbf{A}_\beta$, which we need to develop the "jump-start" procedure, may be a tricky problem almost equivalent to the original spectral problem. On the other hand, if the *approximate* resonance factor $\mathbf{S}_0^\beta$ is used instead the the exact factor, then the division of the scattering matrix through $\mathbf{S}_0^\beta$ would not eliminate singularity, hence the complementary factor of the scattering matrix would be still non-analytic at the origin and hence could not be obtained via analytic perturbation procedure.

6. *Quantum Graph with resonance vertices*

In Section 4 we already discussed the possibility of replacement of the scattering problem for the quantum network by the corresponding energy-dependent Sturm-Liouville problem on the star-shaped quantum graph with the energy-dependent boundary at the vertex, see (27). When substituting the quantum network by the quantum graph one often chooses the standard Kirchhoff-type boundary condition at the nodes, see for instance [**11**, **14**, **21**]. The nearest non-trivial alternative to this simplest choice in our scheme is the energy-dependent boundary condition which corresponds to the inner structure with a single resonance eigenvalue of the intermediate operator on the essential spectral interval. We will calculate these boundary conditions assuming that the corresponding one-pole approximation of the scattering matrix is known. For the quantum network consisting of a single wire with a resonance vertex the model is described by Theorem 5·1. Then, eliminating the inner variables, we obtain for the outer component of the wave-function the Schrödinger equation on the quantum graph with the boundary condition containing the spectral parameter $p^2 = \lambda - \pi^2/2\mu^\perp\delta^2 - V$. Naturally this boundary condition depends on the trajectory of the resonance $k_0(\beta)$ approaching k_0 associated with the resonance eigenvalue $\lambda_0 = k_0^2 + \pi^2/2\mu^\perp\delta^2 + V$ of the intermediate operator when the coupling constant β weakens: $\beta \to 0$:

$$-u'' = p^2 u,\ 0 < x < \infty,$$

$$u'(0) = \left[\beta_{00} - \beta_{01}\frac{\mathcal{M}(\lambda)}{1+\beta_{11}\mathcal{M}(\lambda)}\beta_{01}\right]u(0). \tag{41}$$

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We replace the Krein function in the boundary condition by the corresponding one-pole approximation as in Theorem 5·1, substituting into it the expressions for the boundary parameters β_{ik} calculated above. Then we obtain:

$$u'(0) = \frac{|k_0(\beta)|^2 - p^2}{2\Im k_0(\beta)} u(0). \tag{42}$$

This boundary condition is defined by the trajectory of the resonance $k_0(\beta)$ in dependence of the small parameter β, and it gives formally the scattered wave on the wire:

$$\Psi(x, p) = e^{-ipx} - \mathbf{S}_0^\beta e^{ipx}.$$

Consider now a star-shaped network formed by few equivalent single-mode wires attached to the vertex domain, with the constant potential V, and the width δ. We also assume that $2\mu^\parallel = 1$ and denote $\lambda = p^2 + \pi^2/2\mu^\perp\delta^2 + V$. Assume that the network is thin (the geometric parameter $(ip)^{-1}\beta_{01}$ in the constructed solvable model is small), the Fermi level is situated in the middle of the first spectral band, and there exists a single simple resonance eigenvalue of the intermediate Hamiltonian on a small essential spectral interval Δ centered at the Fermi lavel. The outer component $e^{-ipx}\nu - \mathbf{S}_0^\beta \nu e^{ipx}$ of the wave function of the corresponding solvable model is a vector-function taking values in E_+. It satisfies the equation

$$-u'' = p^2 u, \ 0 < x < \infty, \tag{43}$$

with an appropriate boundary condition at the origin connecting the boundary data in the outer space $u(0), \ u'(0) \in E_+$ with the boundary data $\vec{\xi}_\pm \in E_+$ in the inner space. The boundary parameter β_{01} is found, based on Theorems 4·1, 4·2. Since the wires are equivalent, and the Fermi level is situated on the first spectral band, the diagonal matrix K_+ is proportional to the unit matrix, and hence we again obtain the solvable model with only one wire but with the multi-dimensional entrance subspace E_+. According to Section 5, a single resonance $k_0(\beta) = \Re k_0(\beta) + i\Im k_0(\beta)$ is observed for small β near to the resonance eigenvalue. Then the corresponding "one-pole" approximation of the scattering matrix is presented in form

$$\mathbf{S}_0^\beta = \frac{[p - k_0(\beta)]\,[p + \bar{k}_0(\beta)]}{[p - \bar{k}_0(\beta)]\,[p + k_0(\beta)]} P_\nu + P_\nu^\perp, \tag{44}$$

with the one-dimensional projection $\nu\rangle\langle\nu := P_\nu$ on the appropriate resonance entrance subspace in E_+ spanned by the resonance entrance vector $\nu = P_+(\partial\varphi_0/\partial n)|P_+(\partial\varphi_0/\partial n)|^{-1}$. Here $P_\nu^\perp = I - P_\nu$. Then, using machinery developed for the single wire with the one-dimensional entrance subspace, we obtain the following result:

THEOREM 6·1. *The outer component of the wave-function of the star-shaped solvable model of the network satisfies the above vector equation* (43) *and the boundary condition on the bottom sections of the wires*:

$$u'(0) = \frac{|k_0(\beta)|^2 - p^2}{2\Im k_0(\beta)} P_\nu u(0). \tag{45}$$

We postpone to forthcoming publications analysis of the jump-start for junctions with multidimensional entrance subspaces E_+ of open channels.

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