

Plasma waves in two-dimensional electron channels: propagation and trapped modes

I.A. Semenikhin ^{1,2}, B.S. Pavlov ^{1,3}, V.I. Ryzhii ¹.

¹ Solid State Computer Laboratory, University of Aizu, Aizu-Wakamatsu 9658580, Japan.

² on leave from the Institute of Physics and Technology RAS, Moscow, 117218, Russia,

³ on leave from the Department of Mathematics, the University of Auckland, Private Bag 92019, Auckland, New Zealand;

Abstract

Plasma waves in two-dimensional electron channels, with a non-trivial geometry and governing electrodes, are described by the hydro-dynamical equations, combined with the Poisson equation for the self - consistent electric potential. If the amplitudes of the oscillations of the velocity, the concentration and the potential, are much smaller than the stationary values of these variables, then the hydrodynamical equation for oscillations can be linearized - transformed to the wave equation on a two-dimensional network. We consider the scattering problem for the wave equation and develop a semi-analytic method for calculation of transmission coefficients through the junction. The formulae have resonance character and may be used for manipulation of plasma waves in 2D networks of electron channels.

PACS numbers: 52.75.-d, 02.90.+p

Keywords: Two dimensional electron channel, Dirichlet-to-Neumann map, scattering

1 Introduction: basic equations

The hydrodynamical analogy was suggested for plasma waves in [1, 2] and was intensely used for analysis for plasma waves in two-dimensional (2D) electron channel, with no governing electrodes, see for instance recent paper [3]. In [4] the hydrodynamic electron transport model is used for description of plasma oscillations in gated 2D channel in high electron mobility transistor (HEMT). Analysis of the spectrum of plasma waves, in particular is applicable also to other HEMT-based terahertz devices, in particular those operating in the tera-hertz (THZ) rank of frequencies, see [5, 6].

In particular, for the device constructed of basic electrodes Γ_r^b , forming a 2D electron channel or even a network on the horizontal plane $S = \{z = 0\}$, and few governing electrodes Γ_s^g situated in the lower or upper half-spaces, the calculation of the plasma current is reduced to the self-consistent calculation of the electric potential, concentration and velocity from the system of three basic equations (1,2,3) below.

1. The three-dimensional Poisson equation, for the electric potential, with the corresponding dielectric constant κ

$$\Delta_3 \varphi = \frac{4\pi e}{\kappa} \delta(z) \Sigma \mathcal{X}_T, \quad (1)$$

and the appropriate boundary conditions $\varphi|_{\Gamma_s^g} = V_s^g$, $\varphi|_{\Gamma_r^b} = V_r^b$ on the basic electrodes. This equation connects the potential φ with the non-zero concentration $\delta(z)\Sigma(x, y, 0, t)$ localized on a 2D electron channel Γ situated on the horizontal plane $S : \{z = 0\}$ between the basic electrodes $\Gamma_r^b \in S$. Here the function \mathcal{X}_Γ is the indicator of the channel on S : $\mathcal{X}_\Gamma(x, y) = 1$, if $(x, y) \in \Gamma$, otherwise $\mathcal{X}_\Gamma(x, y) = 0$.

2. The continuity equation connects the concentration Σ and the velocity u of electrons on the 2D electron channel:

$$\frac{\partial \Sigma}{\partial t} + \text{div}_2 \Sigma u = 0, \quad (x, y) \in \Gamma. \quad (2)$$

3. Euler equation for the velocity u on the 2D electron channel:

$$\frac{\partial u}{\partial t} + \langle u, \nabla_2 \rangle u = \frac{e}{m} \nabla_2 \varphi - \nu u, \quad (x, y) \in \Gamma. \quad (3)$$

Representing the concentration, the potential and the velocity in the form of a sum of the stationary value and a harmonic wave process with frequency-dependent amplitudes:

$$\begin{aligned} \varphi(x, z, t) &= \varphi_0(x, y, z) + \int \varphi_\tau(x, y, z) e^{i\tau t} d\tau, \\ \Sigma(x, y, 0, t) &= \Sigma_0(x, y) + \int \Sigma_\tau(x, y) e^{-i\tau t} d\tau, \\ u(x, y, 0, t) &= u_0(x, y, 0) + \int u_\tau(x, y) e^{i\tau t} d\tau, \end{aligned}$$

we linearize the initial basic equations, reducing them to the search of solutions of the non-linear stationary equations

$$\text{div}_2 \Sigma_0 u_0 = 0, \quad \langle u_0, \nabla_2 \rangle u_0 = \frac{e}{m} \nabla_2 \varphi_0 - \nu u_0, \quad \Delta_3 \varphi_0 = \frac{4\pi e}{\kappa} \Sigma_0 \delta(z) \mathcal{X}_\Gamma, \quad (4)$$

with appropriate boundary conditions, and linear equations for the amplitudes of the harmonic wave processes $u_\omega, \Sigma_\omega, \varphi_\omega$:

$$\begin{aligned} -i\omega \Sigma_\tau(x) + \text{div}_2 [\Sigma_0(x, y) u_\tau + u_0(x, y) \Sigma_\tau] &= 0, \\ \Delta_3 \varphi_\tau = \frac{4\pi e}{\kappa} \Sigma_\tau \delta(z) \mathcal{X}_\Gamma, \quad (\nu + i\tau) u_\tau = \frac{e}{m} \nabla_2 \varphi_\tau, \end{aligned} \quad (5)$$

with zero boundary conditions on the electrodes. According to the Poisson equation the jump of the normal derivatives of the stationary potential φ_0 and the corresponding amplitude φ_τ on the 2D electron channel is calculated as $\left[\frac{\partial \varphi_0}{\partial n} \right] = \frac{4\pi e}{\kappa} \Sigma_0$, $\left[\frac{\partial \varphi_\tau}{\partial n} \right] = \frac{4\pi e}{\kappa} \Sigma_\tau$.

Under natural assumptions the linear system (5) may be simplified and, eventually, reduced to the wave equation for the spectral component φ_τ on the 2D electron channel with zero boundary conditions. For instance, under assumption that the concentration and the speed are slowly varying along the streamlines of the stationary speed u_0 , the jump of the normal derivative of the harmonic component of the potential was calculated in [7] as

$$\left[\frac{\partial \varphi_\tau}{\partial n} \right] = \frac{2}{q} \text{div}_2 \Sigma_0(x, y) \nabla_2 \varphi_\tau, \quad (6)$$

with $\frac{2}{q} = \frac{4\pi e^2}{i\tau m \kappa (\nu + i\tau)}$. Generally the expression in the left side of (6) is represented as a combination of Dirichlet-to-Neumann maps on the 2D electron channel $\left[\frac{\partial\varphi_\tau}{\partial n}\right] = -\Lambda_- - \Lambda_+$, where the normal in the jump is directed upward on the 2D electron channel and the DN-maps are defined in a standard way based on the outward normal.

Hereafter we consider the case of the planar basic electrodes $\Gamma_r^b \subset S$, where $S = (z = 0)$. The governing electrodes Γ_s^g are also situated on the planes S_\pm parallel to S , $\text{dist}(S_\pm, S) = W_\pm$, so that the structure of the system of planes \mathfrak{S}_\pm, S constitutes a flat condenser. Then, for the potential $\varphi_\tau(x, y, z)$ vanishing on S_\pm the jump of the normal derivative on the 2D electron channel is usually substituted, see [?, 4], with a negligible error, by the value of the potential $\varphi_\tau(x, y, 0)$

$$\left[\frac{\partial\varphi_\tau}{\partial n}\right] = -\varphi_\tau(x, y, 0) (W_+^{-1} + W_-^{-1})$$

Then the equation for the amplitude $\varphi_\omega(x, y, 0)$ of the harmonic component of the potential on the 2D electron channel is presented in form:

$$(W_+^{-1} + W_-^{-1}) \frac{q}{2} \varphi_\tau(x, y, 0) + \text{div}_2 \Sigma_0(x, y) \nabla_2 \varphi_\tau(x, y, 0). \quad (7)$$

The expression

$$(W_+^{-1} + W_-^{-1}) \frac{q}{2} = (W_+^{-1} + W_-^{-1}) \frac{i\tau m \kappa (\nu + i\tau)}{4\pi e^2}$$

is a symbol of the differential operator

$$m \kappa \frac{W_+^{-1} + W_-^{-1}}{4\pi e^2} \left[\frac{\partial^2}{\partial t^2} + \nu \frac{\partial}{\partial t} \right]$$

In case of trivial geometry of the channel, when the concentration Σ_0 is constant, the coefficient $4\pi e^2 (m \kappa)^{-1} \Sigma_0 [W_+^{-1} + W_-^{-1}]^{-1} := a_0^2$ plays a role of the square of velocity of plasma waves in the device. In general case we also interpret the ratio

$$\frac{4\pi e^2 \Sigma_0(x, y)}{m \kappa (W_+^{-1} + W_-^{-1})} = a^2(x, y)$$

as a square of the local speed $a^2(x, y)$ of plasma waves in the device and rewrite the equation for the potential on the 2D electron channel

$$\varphi(x, y, z, t) - \varphi_0(x, y, z) \Big|_{z=0} = \int \varphi_\tau(x, y, 0) e^{i\tau} d\tau := \varphi_\Gamma(x, y)$$

as

$$\frac{\partial^2 \varphi_\Gamma}{\partial t^2} + \nu \frac{\partial \varphi_\Gamma}{\partial t} = \text{div}_2 a^2(x, y) \nabla_2 \varphi_\Gamma = -\mathcal{L}_a \varphi_\Gamma, \quad x, y \in \Gamma \quad (8)$$

with zero boundary conditions on the boundary of the 2D electron channel. Generally we may assume that the 2D electron channel is just a network Ω of straight plasma channels - the *leads* ω^m - and vertex domains Ω_s on the plane S_0 squeezed between the edges of few basic electrodes Γ_r^b , see for instance (1) We assume that the equilibrium values of concentration,

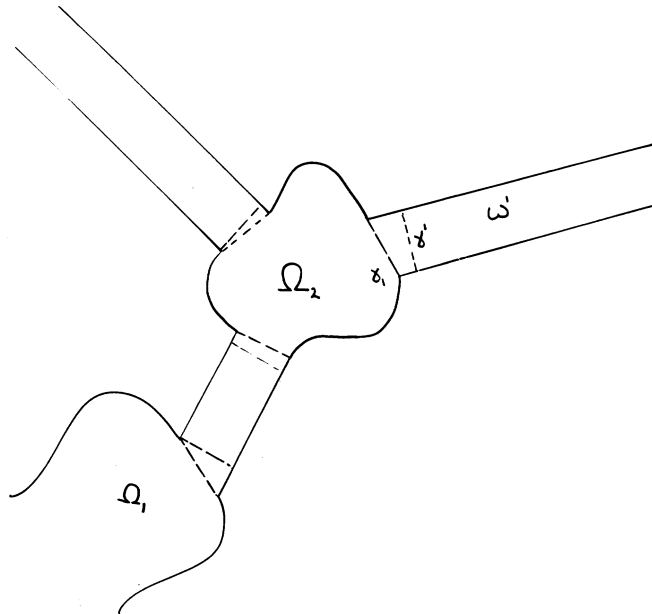


Figure 1: A network of plasma channels

the velocity and the potential are obtained via solution of the system (5). We guess that the local velocity of plasma waves on the leads ω^m is constant, $a(x, y) = a_0$, on the vertex domains Ω_s the velocity is a positive continuous function $a(x, y) = a_s(x, y)$, and all leads have the same width δ . Then essential transport properties of the network Ω can be recovered from the solution of the corresponding scattering problem and represented in form of a table of transmission coefficients across the star-shaped elements- junctions, each of them consisting of a vertex domain and few semi-infinite leads attached to it, see (2). We will develop a semi-analytic method for calculation of scattering matrix of the junction for plasma waves described by (8). In particular, we will calculate the resonances and the resonance states which can be interpreted as trapped modes on the junction, see for instance the recent paper ([8]) and references therein. In this paper we focus on the computational aspects of the scattering problem.

2 Scattering of plasma waves by the junction

Consider a junction $\Omega = \Omega_{int} \cup \omega$ of 2D electron channels constructed of a 2-dim compact vertex domain Ω_{int} on a plane S_0 and several channels - leads $\omega = \cup_m \omega^m$ separated from the junction by imaginable orthogonal bottom sections γ_s , $\cup_s \gamma_s = \gamma$. We assume that all leads have the same width δ . On the junction $\Omega := \Omega_{int} \cup \omega$ we consider the wave-equation for the potential $\varphi_\Gamma := \varphi|_\Gamma$:

$$\frac{\partial^2 \varphi_\Gamma}{\partial t^2} + \nu \frac{\partial \varphi_\Gamma}{\partial t} = \text{div}_2 a^2(x, y) \nabla_2 \varphi_\Gamma. \quad (9)$$

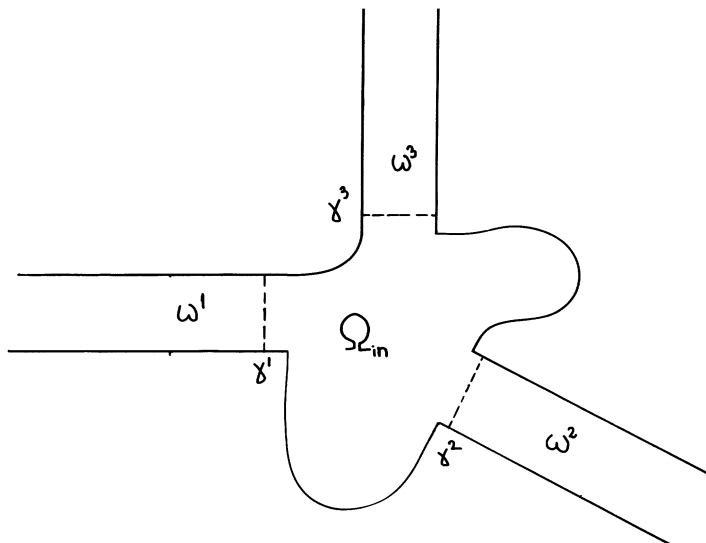


Figure 2: A junction

We assume that the speed $a(x, y)$ is constant on ω , $a(x, y) = a_0$ if $x > 0$. Transport properties of the junction Ω are essentially described by the solutions of the scattering problem for the stationary wave equation

$$\mathcal{L}\varphi_p = p^2\varphi_p = \lambda\varphi_p, \quad (10)$$

The temporal part of the non-stationary wave equation (9) contains the first derivative with a positive coefficient ν which defines dissipation. The spectral parameter p^2 of (10) is connected to the frequency τ by the dispersion relation $i\tau(i\tau + \nu) + p^2 = 0$, or $\tau = \tau(p)$,

$$\tau(p) = i\nu/2 \pm \sqrt{p^2 + \nu^2/4}.$$

Spectrum of the above problem (10) consists of absolutely continuous branches σ_a and contains a countable number of positive embedded eigenvalues λ_s accumulating at infinity. If all leads have the same width δ , the branches are $[a_0^2\pi^2l^2/\delta^2, \infty)$, $l = 1, 2, \dots$, with multiplicity equal to the number of leads attached to the vertex domain Ω_{int} of the junction.

Transport properties of the junction are essentially defined by resonances - the complex poles of the corresponding scattering matrix, see next section, and by the shape of the corresponding resonance states- non-square integrable solutions φ_p of the stationary equation (10) with complex p , $\Im p < 0$. The resonances will be found in section 4 as zeros of the scattering matrix of the junction. Physically the resonance states can be interpreted as a result of breeding of the standing waves in the vertex domain Ω_{int} with the running waves in the leads ω . Search of resonances is a difficult problem of the spectral analysis, which can't be solved by methods of the self-adjoint theory. We will discuss this problem in details in section 3. Resonance solutions of the non-stationary wave-equation are represented as

$$e^{i\tau(p)t}\varphi_p = e^{-\nu/2t} e^{\pm i\sqrt{p^2 - \nu^2/4}} \varphi_p,$$

are exponentially growing in the leads and exponentially decreasing on the vertex domain when $t \rightarrow \text{infy}$, with the rate depending on the position of the resonance and the magnitude of ν .

We proceed with spectral analysis of the self-adjoint problem (10), assuming that the equilibrium velocity $a(x, y)$ is already obtained by straightforward computing. The computed stationary speed $a(x, y)$ tends rapidly to the constant a_0 in the leads, so that choosing the bottom sections properly, we may assume $a(x, y) = a_0$ in ω and is positive and continuous everywhere. We describe the transport properties of the junction via solution of the scattering problem for the wave equation

$$\mathcal{L}\psi = p^2\psi \quad (11)$$

with zero boundary condition on the whole boundary of the junction. On the non-perturbed parts of the 2D electron channel- on the leads - the corresponding spectral problem admits separation of variables, based on the cross-section eigenfunctions $e_l = \sqrt{2/\delta} \sin \pi l y \delta^{-1}$. The scattered waves of the above stationary wave equation (10) in the leads are combined of exponential modes

$$\begin{aligned} e^{\pm i\sqrt{p^2 - \pi^2 l^2 a_0^2 \delta^{-2}} x} e^l &:= \chi_{\pm}^l, \quad p^2 - \pi^2 l^2 a_0^2 \delta^{-2} > 0, \\ e^{\pm \sqrt{\pi^2 l^2 a_0^2 \delta^{-2} - p^2} x} e^l &:= \xi_{\pm}^l, \quad p^2 - \pi^2 l^2 a_0^2 \delta^{-2} < 0. \end{aligned} \quad (12)$$

For any positive $p > a_0\pi/\delta$ there exist a finite number of oscillating modes which correspond to *open spectral canals* on the leads $p^2 - \pi^2 l^2 a_0^2 \delta^{-2} > 0$, and an infinite number of exponentially decreasing (growing) modes $p^2 - \pi^2 l^2 a_0^2 \delta^{-2} < 0$ associated with *closed spectral canals*. The scattering Ansatz

$$\psi_l^m(x) = \begin{cases} \chi_+^l(x) + \sum_{\pi^2 r^2 / \delta^2 < \lambda} S_{l,r}^{m,m} \chi_-^r(x) & + \sum_{\pi^2 r^2 a_0^2 / \delta^2 > \lambda} s_{l,r}^{m,m} \xi_-^r(x), \quad x \in \omega^m \\ \sum_{\pi^2 r^2 a_0^2 / \delta^2 < \lambda} S_{l,r}^{m,n} \chi_-^r(x) & + \sum_{\pi^2 r^2 a_0^2 / \delta^2 > \lambda} s_{l,r}^{n,m} \xi_-^r(x), \quad x \in \omega^n, \quad n \neq m. \end{cases} \quad (13)$$

is bounded and satisfies the stationary equation (10) on the exterior part $\omega = \cup_m \omega^m$ of the junction. Matching the scattering Ansatz $\vec{\psi}$ to the solution of the stationary wave equation $L_{int}\psi = p^2\psi$ on the vertex domain Ω_{int} , we are able, in principle, to define all coefficients of the Ansatz, $S_{l,r}^n, s_{l,r}^n$, see for instance [9]. This infinite linear system can be solved, if the Green - function G_{int} of the Schrödinger equation on Ω_{int} with zero boundary condition on $\partial\Omega_{int}$ is constructed. Really, according to general theory of the second order linear equations, see [10], on the bottom sections the solution u and the boundary current $\frac{\partial u}{\partial n}$ of the boundary problem with data $u|_{\gamma} = u_{\gamma}$ is represented by the integral map with the Poisson kernel

$$\mathcal{P}_{int}(x, \gamma) = -\frac{\partial G_{int}(x, \gamma)}{\partial n} :$$

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

The integral operator \mathcal{DN}_{int} is called ‘‘Dirichlet-to-Neumann map’’, see [11, 12]. It depends on $\lambda = p^2$ and is analytic with poles at the eigenvalues of the Schrödinger operator L_{int}

on the inner part of the network, with zero boundary conditions on $\partial\Omega_{int}$. The coefficients of the scattering Ansatz can be, in principle, found from the infinite linear system which obtained by substitution of the scattering Ansatz into

$$\left. \frac{\partial\psi}{\partial n} \right|_{\gamma} = \mathcal{DN}_{int}\psi \Big|_{\gamma}. \quad (14)$$

To derive the formula for the scattering matrix in terms of \mathcal{DN}_{int} for given value $\lambda = p^2$ of the spectral parameter, we introduce *the entrance suspaces* of the open and closed canals.

$$E_+ = \bigvee_{p^2 - \pi^2 l^2 a_0^2 \delta^{-2} > 0} e_l, \quad E_- = \bigvee_{p^2 - \pi^2 l^2 a_0^2 \delta^{-2} < 0} e_l,$$

and denote by P_{\pm} the corresponding projections, $P_+ + P_- = I$, $E_+ \oplus E_- = E := L_2(\Gamma)$. Represent the restriction of the DN-map of L_{int} by 2×2 operator matrix with matrix elements $\mathcal{DN}_{\pm, \pm'} = P_{\pm} \mathcal{DN} P_{\pm'}$

$$\mathcal{DN}_{int} = \begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix}. \quad (15)$$

Then, denoting by K_+ , K_- the exponents of the modes in (12) in E_+ , E_-

$$K_+(p) := \sum_{p^2 - \pi^2 l^2 a_0^2 \delta^{-2} > 0} \sqrt{p^2 - \pi^2 l^2 a_0^2 \delta^{-2}} e_l \langle e_l,$$

$$K_-(p) := \sum_{p^2 - \pi^2 l^2 a_0^2 \delta^{-2} < 0} \sqrt{\pi^2 l^2 a_0^2 \delta^{-2} - p^2} e_l \langle e_l,$$

and by \mathcal{M} the aggregat (to be interpreted later),

$$\mathcal{M}(\lambda) := \mathcal{DN}_{++} - \mathcal{DN}_{+-} \frac{I}{\mathcal{DN}_{--} + K_-} \mathcal{DN}_{-+}, \quad (16)$$

we obtain the scattering matrix of the pair $(\mathcal{L}, l^{\omega})$ in a form of ratio:

$$S(p) = [iK_+(p) + \mathcal{M}(\lambda)]^{-1} [iK_+(p) - \mathcal{M}(\lambda)], \quad (17)$$

see [13, 14].

3 Scattering matrix via Intermediate DN map

The above standard method of calculation of the scattering matrix gives not only the scattering matrix S , but also excessive information on coefficients s in front of the evanescent modes. In fact only the information on asymptotic behavior of the oscillating part of the scattered waves, encoded in the scattering matrix, defines the transport properties of the junction. But the standard method is unable to produce the scattering matrix separately from coefficients in front of evanescent modes. Necessity to calculate the coefficients in front of these modes makes the problem much more difficult. In [13] a modified approach

to calculation of the scattering matrix was proposed, which permits to eliminate evanescent waves due to choosing the unperturbed operator in different way.

Indeed, the classical choice of the unperturbed operator as a splitting $\{L_{int} \oplus l^\omega\}$ defined by “the solid wall” on γ (zero boundary conditions) involves additional difficulties because, firstly, this perturbation is infinite-dimensional and, secondly, because of infinite number embedded eigenvalues of L_{int} sitting on the absolutely-continuous spectrum of l^ω . When we remove the solid wall, replacing the zero boundary conditions by the matching condition, we introduce very strong perturbation, which causes breeding of the running waves in the open canals of ω with the standing waves on the vertex domain Ω_{int} of the junction. This breeding transforms embedded eigenvalues of L_{int} into resonances. Classical methods of the selfadjoint perturbation theory are unable to describe this transformation for infinite-dimensional perturbations. But we are able to modify the analytic perturbation technique, see for instance [13, 14], choosing another unperturbed operator so that *the perturbation becomes finite-dimensional*. Then the transformation of the embedded eigenvalues into resonances can be treated by finite-dimensional technique and the calculation of the scattering matrix is reduced to solution of an algebraic equation.

We are able to fulfil the described program restricting our analysis onto selected essential spectral interval Δ centered at some spectral point Λ_0 :

$$\Delta = [\Lambda_0 - \varepsilon, \Lambda_0 + \varepsilon],$$

with *no spectral thresholds on Δ* , hence with constant multiplicity of the continuous spectrum of l^ω . The essential spectral interval can be interpreted as a sensitivity range of the device which is used in course of observation of the scattering of waves in the 2D channel.

We consider the decomposition of $L_2(\gamma)$ into the orthogonal sum of the *entrance subspaces* of the open and closed canals, with respect to Λ_0 :

$$L_2(\gamma) = \bigvee_{\frac{\pi^2 a_0^2 l^2}{\delta^2} < \Lambda_0} e_l \oplus \bigvee_{\frac{\pi^2 a_0^2 l^2}{\delta^2} > \Lambda_0} e_l =: E_+^0 \oplus E_-^0.$$

Denote by P_\pm^0 the corresponding orthogonal projections $P_+^0 + P_-^0 = I$. The exponential modes of the wave equation in the 2D channel, spanned by the elements e_l from the subspace E_+^0 , are oscillating on Δ , and ones spanned by elements e_l from E_-^0 , are evanescent modes. We separate them by introducing “the partial zero boundary condition”

$$P_+^0 u \Big|_\gamma = 0, \tag{18}$$

which is a softer perturbation, than the solid wall. By imposing the additional boundary condition (18) the operator \mathcal{L} is split into an orthogonal sum of the unperturbed operator l^0 on the leads $E_+^0 \times L_2(0, \infty) = \mathcal{H}^0$

$$l^0 = -\frac{d^2}{d(x^\parallel)^2} P_+ + \sum_{open} [\pi^2 l^2 \Sigma_0 \delta^{-2}] e_l \langle e_l,$$

and a selfadjoint operator L^0 in the orthogonal complement $L_2(\Omega \cup \omega) \ominus \mathcal{H}_+$:

$$\mathcal{L} \longrightarrow \mathcal{L}^0 = l^0 \oplus L^0.$$

The continuous spectrum of \mathcal{L} is split accordingly: the “open” branches $\sigma_l = [\frac{\pi^2 a_0^2 l^2}{\delta^2}, \infty)$, $\frac{\pi^2 a_0^2 l^2}{\delta^2} < \Lambda_0$ are inherited by l^0 , and the “closed” branches $\sigma_l = [\frac{\pi^2 a_0^2 l^2}{\delta^2}, \infty)$, $\frac{\pi^2 a_0^2 l^2}{\delta^2} > \Lambda_0$ are inherited by L^0 . The “softer” - finite-dimensional- perturbation defined by (18) was suggested in [13, 15]. It appeared, see [14], that it gives a geometrical interpretation of the phenomenological Datta condition at the junction of a one-dimensional network, [16, 17, 18].

The boundary condition (18) defines a *semi-transparent wall* at γ which neither admits to Ω_{int} the waves from the open spectral canals in the leads, nor releases the waves from Ω_{int} , shaped on γ to fit open spectral canals, to exit from Ω to ω . We refrain here from a discussion of a physical realization of this boundary condition, but we remark, that, due to the finite dimension of E_+ , the perturbation in \mathcal{L} introduced by the additional boundary condition (18) is finite-dimensional. The operator L^0 has a finite number of eigenvalues below $\lambda_{min} = \min_{\pi^2 a_0^2 l^2 / \delta^2 > \Lambda_0} \pi^2 a_0^2 l^2 / \delta^2$ and probably a countable number of embedded eigenvalues accumulating at infinity. The eigenvalues situated below the lower threshold $\lambda_{min} =: \pi^2 a_0^2 l_{min}^2 \delta^{-2}$ play an important role in scattering processes, [15]. When the semi-transparent wall is removed, they are transformed to resonances, which define the transport properties of the junction.

The operator L^0 plays hereafter a role of the *intermediate Hamiltonian*. We are able to obtain the Green function G^0 of L^0 , for $\lambda < \lambda_{min}$, and other spectral characteristics on that interval, via modified analytic perturbation procedure from the corresponding characteristics of L_{int} . Once the Green function G^0 is known, we are able to construct the corresponding Poisson map solving the intermediate boundary problem with data $u_\gamma \in E_+^0$:

$$u_\gamma(x) = \int_\gamma \mathcal{P}^0(x, \gamma) u_\gamma(\gamma) d\gamma, \quad x \in \Omega_{int},$$

with the kernel $\mathcal{P}^0(x, \gamma) = -\frac{\partial G^0(x, \gamma)}{\partial n}$, and the corresponding DN-map:

$$P_+^0 \frac{\partial u}{\partial n} \Big|_\gamma = -P_+^0 \int_\gamma \frac{\partial^2 G^0(x, \gamma)}{\partial n_x \partial n_\gamma} u_\gamma(\gamma) d\gamma \Big|_\gamma =: \mathcal{DN}^0 u_\Gamma.$$

The use of \mathcal{DN}^0 simplifies the problem of matching, because all matrix coefficients $s^{m,n}$ in front of the evanescent modes are taken into account automatically by the solution of the intermediate boundary problem. But even more: if we introduce into (17) the exponentials K_\pm^0 corresponding to the decomposition $E = E_+^0 \oplus E_-^0$, then the cumbersome aggregate \mathcal{M} which appeared in the above expression (17) for the scattering matrix just coincides with \mathcal{DN}^0 . Thus the formula (17) for the scattering matrix can be represented as

$$S(p) = [iK_+^0(p) + \mathcal{DN}^0]^{-1} [iK_+^0(p) - \mathcal{DN}^0]. \quad (19)$$

DN-map $\mathcal{DN}^0(\lambda)$ of the intermediate Hamiltonian L^0 is a sophisticated object: it contains a sum over the eigenvalues of L^0 and an integral over its continuous spectrum, see [15, 14]. But the structure of it on the essential interval of the spectral parameter Δ situated below the lower threshold λ_{min} of the continuous spectrum, is simpler: it can be represented as a sum of polar terms over the eigenvalues of the intermediate operator on Δ :

$$\sum_{\lambda_s \in \Delta} \frac{P_+ \frac{\partial \varphi_s^0}{\partial n} \langle P_+ \frac{\partial \varphi_s^0}{\partial n} |}{\lambda - \lambda_s^0} =: \mathcal{DN}_\Delta^0$$

and a regular function \mathcal{K}_Δ^0 on a complex neighborhood Ω_Δ :

$$\mathcal{DN}^0 = \mathcal{DN}_\Delta^0 + \mathcal{K}_\Delta^0.$$

If the leads ω are thin, and the essential spectral interval Δ is selected in the middle of the interval $(\lambda_{max}, \lambda_{min})$ between the upper threshold of the open channels $\max_{\pi^2 a_0^2 l^2 / \delta^2 < \Lambda_0} \pi^2 a_0^2 l^2 / \delta^2 = \lambda_{max} =: \pi^2 a_0^2 l_{max}^2 / \delta^2$ and the lower threshold of the closed channels, then $K_+^0 \approx \sqrt{\Lambda_0 - \lambda_{max}} \approx \pi a_0 l_{max} \delta^{-1}$ is large and can even dominate the error \mathcal{K}^0 of the above rational approximation on the essential spectral interval:

$$|K_+^0(\lambda)| \gg \max_{\lambda \in \Omega_\Delta} |\mathcal{K}_\Delta^0|, \quad \lambda \in \Omega_\Delta. \quad (20)$$

Then the expression (19) for the scattering matrix can be replaced on Ω_Δ by the simpler expression:

$$S(p) \approx S_{approx}(p) = [K_+^0(p) - \mathcal{DN}_\Delta^0]^{-1} [K_+^0(p) + \mathcal{DN}_\Delta^0], \quad (21)$$

where the correcting term \mathcal{K}^0 is neglected. For thin networks the exact scattering matrix can be obtained from S_{approx} by the geometrically convergent analytic perturbation series, see [13]. The approximate scattering matrix of the junction can be interpreted, see [20] as the scattering matrix of an explicitly solvable model of the junction, represented as a star-shaped graph with an inner space $\bigvee_{\lambda_s \in \Delta} \varphi_s =: E^\Delta$ attached to the node and supplied with an "inner Hamiltonian" -

$$L_\Delta^0 := \sum_{\lambda_s^0 \in \Delta} \lambda_s^0 \varphi_s^0 \langle \varphi_s^0,$$

which is just a part of the intermediate Hamiltonian in E^Δ . The boundary conditions at the node are defined, see [20], such that the scattering matrix of the model coincides on the essential spectral interval, with a good precision with the approximate scattering matrix, so that the constructed model is *fitted*. The resonances of the solvable model situated near the continuous spectrum (in Ω_Δ) can be found as solutions of the algebraic equation $[K_+^0(p) + \mathcal{DN}_\Delta^0(\lambda)]e_\lambda = 0$. For thin junctions they are situated close to the resonances of the original operator \mathcal{L} , see [21], and thus define the resonance character of transport properties of the junction, in particular, the speed of transition properties when the junction is manipulated by an exterior electric field, arising from additional potentials on the governing electrodes Γ^g , or by changing details of the geometry of the junction.

It follows from the above arguments, that the intermediate Hamiltonian plays an important role in the developed theory: it essentially defines the transport properties of the junction on the essential spectral interval, see an extended discussion in [22]. That's why calculation of the spectral characteristics of the intermediate Hamiltonian is important. Unfortunately, the corresponding spectral problem is not a standard problem of spectral analysis, so there is no standard software for computing eigenfunctions and eigenvalues of it. In [19] a special perturbation technique is developed to calculate the Dirichlet-to-Neumann map of the the intermediate Hamiltonian L^0 based on spectral characteristics of the spectral data of the corresponding operator L_{int} on the vertex domain Ω_{int} . It appeared that, essentially, the spectral characteristics of L^0 can be substituted, for thin junctions, by the spectral characteristics of L_{int} , More precise, the result achieved in [19] can be represented in the following form.

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

$$\mathcal{DN} = \mathcal{DN}^\Delta + \mathcal{K} \quad (22)$$

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

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

Due to the spectral representation of the \mathcal{DN} , we have

$$\mathcal{DN}_{+-}^\Delta = \sum_{\lambda_s \in \Delta_T} \frac{P_+ \frac{\partial \varphi_s}{\partial n} \langle P_- \frac{\partial \varphi_s}{\partial n} |}{\lambda - \lambda_s}, \quad (23)$$

where φ_s are the eigenfunctions of L_{int} on Δ . We introduce also the linear hull $E^\Delta = \bigvee_s \{\varphi_s\}$ - an invariant subspace of L_{int} corresponding to the essential spectral interval Δ and the part $L^\Delta := \sum_{\lambda_s \in \Delta} \lambda_s \varphi_s \langle \varphi_s |$ of L_{int} in the invariant subspace E^Δ . To calculate the intermediate DN-map

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

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

$$[\mathcal{K}_{--} + K_-]^{-1} \quad (25)$$

exists on Δ . Using the large parameter K_- , we are able to develop an analytic perturbation procedure for the denominator in the Krein formula. Denote by \mathcal{T} the map

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

and introduce

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

and

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

The perturbation procedure permits to observe the compensation of singularities in Krein formula for \mathcal{DN}^0 inherited from L_{int} and represent the formula for it in more convenient form.

Theorem on compensation of singularities [19] *If the condition (25) is fulfilled on the essential spectral interval Δ then the intermediate DN-map can be represented, by a finite matrix $\dim E_+ \times \dim E_+$ on the essential spectral interval Δ as*

$$\mathcal{DN}^0 = \mathcal{K}_{++-}$$

$$-\mathcal{K}_{+-} \frac{I}{\mathcal{K}_{--} + K_-} \mathcal{K}_{-+} + P_+ \mathcal{J} \mathcal{T}^+ \rangle \frac{I}{\lambda I - L^\Delta + Q(\lambda)} \langle \mathcal{T} \mathcal{J}^+ P_+, E_+ \rightarrow E_+. \quad (26)$$

We call the above representation (26) *the modified Krein formula* for the intermediate DN-map.

For thin junctions the first addendum of the intermediate DN-map

$$\mathcal{K}_{++} - \mathcal{K}_{+-} \frac{I}{\mathcal{K}_{--} + K_-} \mathcal{K}_{-+}$$

in the formula (19) can be neglected, compared with K_+ , so that we obtain a modified expression for the approximate scattering matrix with the polar term only

$$P_+ \mathcal{J} \mathcal{T}^+ \rangle \frac{I}{\lambda I - L^\Delta + Q(\lambda)} \langle \mathcal{T} \mathcal{J}^+ P_+ = \mathcal{M}^\Delta : \\ S_{approx}(p) = [iK_+ + \mathcal{M}^\Delta]^{-1} [iK_+ - \mathcal{M}^\Delta]. \quad (27)$$

Then the *thin* junction of 2D electron channels can be substituted, for theoretical analysis, by the corresponding solvable model, based on results of [19]. The aim of this paper is: search for an adequate computing for spectral quantities of an *arbitrary junction* and for the DN-map of the intermediate Hamiltonian.

4 Direct computing for the Intermediate Hamiltonian

Calculation of eigenvalues and eigenfunctions of the intermediate hamiltonian is a non-standard problem of computational spectral analysis. Up to now, we did not have any standard programs to compute the spectral quantities of the intermediate Hamiltonian. That's why in [14, 22] analysis is based on a special analytic perturbation techniques.

In this section we suggest a semi-analytic method for calculation transport properties of the junction, based on straightforward computing for spectral quantities of the intermediate operator. Note in this connection the recent paper [23], where an efficient computational technique is developed for junctions based on classical ideas. The objects considered in [23] are infinite-dimensional. The method suggested by the authors of [23] proves to be efficient due to use of an additional boundary condition $u \Big|_{\gamma} \perp E_+$ at the final stage of computation.

This condition in fact coincides with our condition imposed onto the eigenfunctions of the intermediate Hamiltonian, see section 2 above, and our papers [13, 14].

In this section we suggest our version of the direct computing for the junction, based on the intermediate Hamiltonian. Our version of computing for the scattering matrix and for resonances deals mainly with finite matrices $\dim E_+ \times \dim E_+$, because the evanescent modes are eliminated via introduction of the Intermediate Hamiltonian. Complete spectral picture of the intermediate Hamiltonian for thin junction is developed in [22], but we know numerous publications where detail of this picture are described, see [24, 25, ?, 27, 28]. The main original part of our result in [22] is the proof of existence of the intermediate Poisson map, which requires extension of the Schwartz theorem on the integral representation of the resolvent, see [29] for the intermediate Hamiltonian, and the connection between the intermediate DN-map and the classical DN-map of the Schrödinger operator in Ω_{int} .

4.1 Eigenvalues of the intermediate Hamiltonian

Note, first of all, that the eigenvalues of the intermediate Hamiltonian for the thin junction can be found as vector zeros of the re-normalized denominator

$$\left[I - L^\Delta + Q(\lambda) \right] e^0 = 0, \quad (28)$$

or, in the original form, for an arbitrary junction:

$$\left[\mathcal{DN}_{--} + K_-^0 \right] e = 0. \quad (29)$$

To solve this equation effectively, we should calculate the DN-map of L_{int} .

Let $\{\varphi_s\}_{s=1}^\infty$, $\{\psi_s\}_{s=1}^\infty$ be orthogonal bases in $L_2(\partial\Omega_{int})$. Following [?], consider two boundary problems for the original differential equation $\mathcal{L}u - \lambda u = 0$, with the Dirichlet and Neumann boundary conditions on $\partial\Omega_{int}$:

$$u \Big|_{\partial\Omega_{int}} = \varphi_s, \text{ and } \frac{\partial u}{\partial n} \Big|_{\partial\Omega_{int}} = \psi_s \quad (30)$$

respectively, assuming that λ is not an eigenvalue of the corresponding homogeneous problems. Denote solutions of this equations by Φ_s^D , Ψ_s^N respectively. Then the integration by parts gives the following formulae :

$$\int_{\Omega_{int}} \nabla_2 \Phi_s a(x, y) \nabla_2 \bar{\Phi}_t dx dy - \lambda \langle \Phi_s, \Phi_t \rangle = a_0^2 \int_{\partial\Omega_{int}} \frac{\partial \Phi_s}{\partial n} \bar{\varphi}_t d\sigma = a_0^2 \langle \mathcal{DN} \varphi_s, \varphi_t \rangle, \quad (31)$$

$$\int_{\Omega_{int}} \nabla_2 \Psi_s a^2(x, y) \nabla_2 \bar{\Psi}_t dx dy = a_0 \int_{\partial\Omega_{int}} \frac{\partial \Psi_s}{\partial n} \bar{\psi}_t d\sigma \lambda \langle \Phi_s, \Phi_t \rangle = a_0^2 \langle \psi_s, \mathcal{ND} \psi_t \rangle. \quad (32)$$

Here \mathcal{ND} is the Neumann-to-Dirichlet map of \mathcal{L} in the domain Ω_{int} , $\mathcal{ND} \times \mathcal{DN} = I$ in the appropriate Sobolev space $W_2^{3/2}(\partial\Omega_{int})$. Since the eigenvalues of the Dirichlet and Neumann problems never coincide, at least one of the above boundary problems has a solution, for given λ , hence either the matrix of \mathcal{DN} , or the matrix of \mathcal{ND} can be found. Then due to $\mathcal{ND} \mathcal{DN} = I$ the DN-map can be calculated near to the eigenvalue of the Dirichlet problem, as the inverse of the ND-map.

The suggested algorithm is practical, see [23] when reducing the above expression for matrix elements of DN and ND maps to the finite matrices $1 \leq s, t \leq N$, if the distance between the eigenvalues of the Dirichlet and Neumann problems are not too small. Then the approximate DN and ND maps are obtained as $N \times N$ matrices. We can use this observation when calculating the intermediate DN-map based on modified analytic perturbation procedure, see [19].

4.2 Search for eigenfunctions/eigenvalues of the intermediate Hamiltonian

Note, first of all, that the spectral problem on discrete spectrum of the intermediate Hamiltonian can be substituted, below the lower threshold $\min_{closed} \pi^2 l^2 a_0^2 \delta^{-2}$ of its continuous spectrum by the “non standard” spectral problem

$$-\nabla_2 a^2(x, y) \nabla_2 \varphi_p = p^2 \varphi_p, \quad P_+^0 \varphi_p \Big|_{\gamma_x, x>0} = 0. \quad (33)$$

for the Schrödinger operator restricted onto the orthogonal complement $L_2(\Omega) \ominus \mathcal{H}_+$ of the open canals $E_+ \times L_2(0, \infty) =: \mathcal{H}_+^0$. Note that the projection $I - P_{\mathcal{H}_+^0}$ generally spoils the continuity of the functions from the domain of \mathcal{L} on the bottom section $\gamma := (x = 0)$. Hence we are not able to rewrite the above spectral problem (33) with $\mathcal{P}^0 := P_{\mathcal{H}_+^0}$ and $\mathcal{P}^\perp := I \ominus P_{\mathcal{H}_+^0}$ in $L_2(\Omega)$ as a problem for the singular “operator” $\mathcal{P}^\perp \mathcal{L} \mathcal{P}^\perp := \mathcal{L}^\perp$ in $L_2(\Omega) \ominus \mathcal{H}_+$. But after the reduction of the operator \mathcal{L} to a finite matrix \mathcal{L}_N , respecting the invariant subspace \mathcal{H}_+ of the splitting, we obtain a bounded operator, hence the multiplication of it by the projection \mathcal{P}^\perp on the left or on the right (or on both sides) is legal. Thus the intermediate spectral problem is reduced, in matrix form, to the selfadjoint spectral problem

$$\mathcal{P}^\perp \mathcal{L}_N \mathcal{P}^\perp \varphi = \lambda \varphi, \quad (34)$$

where φ is an N -component vector. Note that the projection factor \mathcal{P}^\perp the right (or left) side may be omitted, if we develop an iteration process for the eigenvectors, restoring the orthogonality to \mathcal{H}_+ on each step. A convenient procedure for calculation of the eigenvector at the lower eigenvalue λ_s^0 of L_0 may be based on the corresponding heat equation $\frac{du}{dt} = \mathcal{P}^\perp \mathcal{L}_N \mathcal{P}^\perp u$,

$$e^{-\tau R^{-1} \mathcal{L}_N} R \varphi \approx \left[\mathcal{P}^\perp (1 - \tau R^{-1} \mathcal{L}_N) \right]^R e^{-\lambda_1 \tau} \varphi \rightarrow \langle \varphi, \varphi_1 \rangle \varphi_1,$$

for large N, R .

In fact, when calculating the scattering matrix of an asymmetric T-junction below, we used slightly modified iteration suggested in [31]. First of all, we do not make use of the basis respecting the invariant subspaces of the intermediate operator, so that each step of iteration may give in a result, which is not orthogonal to the subspace \mathcal{H}_+ . Secondly, instead of iteration of the aggregat arising from the heat equation, we consider, for the fixed grid, see [30], the discretized operator $\mathcal{L}^N =: \mathbf{H}$ and select the value λ of the spectral parameter equal to the maximal eigenvalue of \mathbf{H} . Then, following [31] and using the corresponding notations, we iterate the operator $\mathbf{M}(\lambda - \mathbf{H})$, applying the projection $\mathbf{M} = I - P^\perp$ onto the orthogonal complement of \mathcal{H}_+ in $L_2(\gamma)$ on each step, because the non-respecting of the invariant subspaces of \mathcal{L} by the basis selected gives, generally, a non-orthogonal to \mathcal{H}_+ result on each step of the iteration. After arranging the iterations in form of a product, we see, that the factors \mathbf{M} may be attached, equivalently, to each factor on the right, as $(\lambda - \mathbf{H})\mathbf{M}$ or on both sides as $\mathbf{M}(\lambda - \mathbf{H})\mathbf{M}$, because $\mathbf{M}^2 = \mathbf{M}$.

4.3 Search for the DN-map of the intermediate Hamiltonian

To find the DN-map of the intermediate Hamiltonian, we should solve the corresponding intermediate boundary problems:

$$\begin{aligned} -\nabla a^2 \nabla u^D &= \lambda u^D, \\ P_+ u^D \Big|_{\gamma_{int}} &= d_\gamma \in E_+, \quad P_+ u^D \Big|_{\gamma_x, x>0} = 0, \end{aligned} \quad (35)$$

, for u^D smoothly extended from Ω_{int} to ω in closed canals. Similar problem for ND-map is

$$-\nabla a^2 \nabla u^N = \lambda u^N,$$

$$P_+ \frac{\partial u^N}{\partial n} \Big|_{\gamma_{int}} = n_\gamma \in E_+, P_+ u^N \Big|_{\gamma_x, x>0} = 0, \quad (36)$$

also for u^N smoothly extended to ω in closed canals. The corresponding intermediate DN and ND maps are introduced as :

$$\mathcal{DN}^0 : d_\gamma \rightarrow P_+ \frac{\partial u^D}{\partial n} \Big|_{\gamma_{int}}, \quad \mathcal{ND}^0 : n_\gamma \rightarrow P_+ u^N \Big|_{\gamma_{int}}.$$

Via integraion by parts in the boundary form

$$\int_\gamma \left[\frac{\partial u^D}{\partial n} P_+ \bar{u}^N - P_+ u^D \frac{\partial \bar{u}^N}{\partial n} \right] d\gamma = 0$$

we derive $\mathcal{ND}^0 \times \mathcal{DN}^0 = P_+ = I_{E_+}$. Hence, similarly to the classical situation, see the subsection 4.1, we can search for one of maps $\mathcal{ND}^0, \mathcal{DN}^0$, and find another one as it's inverse.

We substitute the above non-standard boundary problem for \mathcal{DN}^0 by the standard boundary problem on Ω_{int} . Separate the basis φ_s into two parts $\varphi_s^\pm \in E_\pm, E_+ \oplus E_- = E$, and construct solutions of the corresponding boundary problems:

$$\begin{aligned} -\nabla a^2 \nabla \Phi_s^\pm &= \lambda \Phi_s^\pm, \\ P_+ \Phi_s^\pm \Big|_{\gamma_{int}} &= \varphi_s^\pm. \end{aligned} \quad (37)$$

The solution of the standard boundary problem

$$-\nabla a^2 \nabla u = \lambda u, \quad u \Big|_{\partial\Omega} = \sum_s u_+^s \varphi_s^+ + \sum_t u_-^t \varphi_t^- =: u_\gamma^+ + u_\gamma^-$$

is represented in Ω_{int} as

$$u = \sum_s u_+^s \Phi_s^+ + \sum_t u_-^t \Phi_t^- =: u^+ + u^-. \quad (38)$$

Consider the matrix of the classical DN- map with respect to the decompositions $E = E_+ \oplus E_-$, with elements $P_+ \mathcal{DN} P_- = \mathcal{DN}_{+-}, \dots$

$$\begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix} =: \mathbf{DN},$$

and denote by $\vec{u}_\gamma, \vec{\rho}_\gamma$, the columns combined of (u_γ^+, u_γ^-) and the corresponding normal derivatives $\left(\frac{\partial u_\gamma^+}{\partial n}, \frac{\partial u_\gamma^-}{\partial n} \right)$. We also denote by \mathcal{M} the diagonal matrix $[\mathcal{DN}_0, -K_-]$. Then, due to smooth continuation of u to ω in closed canals we have the equation for \mathcal{DN}_0

$$\mathbf{DN} \vec{u}_\gamma = \vec{\rho}_\gamma = \mathcal{M} \vec{u}_\gamma. \quad (39)$$

Solving this equation we obtain the representation of \mathcal{DN}_0 as a Shur complement

$$\mathcal{DN}_0 = \mathcal{DN}_{++} - \mathcal{DN}_{+-} \frac{I}{\mathcal{DN}_{--} + K_-} \mathcal{DN}_{-+}.$$

Note that matrix elements of each detail of the formula can be obtained based on the bi-linear formula 31.

Similar construction gives the intermediate ND-map in terms of matrix elements of the decomposition

$$\begin{pmatrix} \mathcal{N}\mathcal{D}_{++} & \mathcal{N}\mathcal{D}_{+-} \\ \mathcal{N}\mathcal{D}_{-+} & \mathcal{N}\mathcal{D}_{--} \end{pmatrix} =: \mathbf{ND}$$

of the classical ND - map with respect to $E_+ \oplus E_-$:

$$\mathcal{N}\mathcal{D}_0 = \mathcal{N}\mathcal{D}_{++} - \mathcal{N}\mathcal{D}_{+-} \frac{I}{K_-^{-1} + \mathcal{N}\mathcal{D}_{--}} \mathcal{N}\mathcal{D}_{-+}.$$

Note that zeros of the intermediate ND-map are the poles of the intermediate DN map and coincide with eigenvalues of the intermediate Hamiltonian. Once intermediate map $\mathcal{N}\mathcal{D}_0$ is calculated, the formula $\mathcal{N}\mathcal{D}_0 \times \mathcal{D}\mathcal{N}_0 = I$ can be used to find another. Numerical realization is stable if the eigenvalues of the corresponding intermediate Dirichlet and Neumann spectral problems are well separated.

4.4 Straightforward computing for the scattering matrix

The above non-spectral approach to the calculations of DN and ND maps permits to calculate the polar terms of the DN-map near and thus gives a possibility to describe the resonance behavior of the scattering matrix near the eigenvalue of the intermediate hamiltonian without formal solution of the spectral problem. The idea of the following calculation belongs to V. Adamyan. We do it here only in the case when the zero λ_1 of the Hermitian matrix $\mathcal{N}\mathcal{D}_0$ is simple and one-dimensional: $\mathcal{N}\mathcal{D}_0(\lambda_1)Q_1 = 0$, with $Q_1 = e_1 \rangle \langle e_1$, and $Q_1^\perp \mathcal{N}\mathcal{D}_0(\lambda_1)Q_1^\perp =: \mathcal{N}\mathcal{D}^{\perp\perp}$ is invertible. Then the matrix $\mathcal{N}\mathcal{D}_0(\lambda)$ is represented near to λ_1 in the orthogonal basis e_1, E_1^\perp as

$$\mathbf{ND}_0 = \begin{pmatrix} d_1(\lambda - \lambda_1) & (\lambda - \lambda_1)\mathcal{N}\mathcal{D}_{1\perp} \\ (\lambda - \lambda_1)\mathcal{N}\mathcal{D}_{\perp 1} & \mathcal{N}\mathcal{D}_{\perp\perp} \end{pmatrix}, \quad (40)$$

with analytic near λ_1 functions $d_1, \mathcal{D}_{1\perp}, \mathcal{D}_{\perp 1}$, $d_1(\lambda_1) \neq 0$ and $\mathcal{N}\mathcal{D}_{\perp\perp}(\lambda)$ calculated by symmetry principle as $\mathcal{N}\mathcal{D}_{+1\perp}(\bar{\lambda})$. Then $\mathcal{D}\mathcal{N}_0$ is also represented, see [32], near λ_1 in form

$$\mathbf{DN}_0 = \begin{pmatrix} d_1^{-1}(\lambda - \lambda_1)^{-1} & \mathcal{D}\mathcal{N}_{1\perp} \\ \mathcal{N}\mathcal{D}_{+1\perp} & \mathcal{D}\mathcal{N}_{\perp\perp} \end{pmatrix} =: d_1^{-1} \frac{Q_1}{\lambda - \lambda_1} + \mathbf{D}, \quad (41)$$

with analytic bounded matrix elements $\mathcal{D}\mathcal{N}_{1\perp}, \mathcal{D}\mathcal{N}_{\perp\perp}$ uniquely defined near λ_1 by $d_1(\lambda_1)$ and the matrices $\mathcal{N}\mathcal{D}_{1\perp}, \mathcal{N}\mathcal{D}_{\perp\perp}$. Hence the scattering matrix near the zero λ_1 of the ND-map is represented as

$$S(\lambda) = \left[iK_+ + \frac{d_1^{-1}(\lambda)Q_1}{\lambda - \lambda_1} + \mathbf{D}(\lambda) \right]^{-1} \left[iK_+ - \frac{d_1^{-1}(\lambda)Q_1}{\lambda - \lambda_1} - \mathbf{D}(\lambda) \right].$$

For thin networks the resonances of the full scattering matrix can be calculated approximately with use of the operator-valued Rouché theorem, [21], based on the approximate scattering matrix

$$S_{approx}(\lambda) = \left[iK_+ + \frac{d_1^{-1}(\lambda_1)Q_1}{\lambda - \lambda_1} + \mathbf{D}(\lambda_1) \right]^{-1} \left[iK_+ - \frac{d_1^{-1}(\lambda_1)Q_1}{\lambda - \lambda_1} - \mathbf{D}(\lambda_1) \right].$$

One more straightforward possibility of using the ND-map is just based on the formula:

$$S(\lambda) = [i\mathcal{N}\mathcal{D}_0 K_+ - I]^{-1} [i\mathcal{N}\mathcal{D}_0 K_+ + I], \quad (42)$$

which is equivalent to (17), since $\mathcal{M} := \mathcal{D}\mathcal{N}_0 = \mathcal{N}\mathcal{D}_0^{-1}$. Choice one of formuls (42, 17) may be more convenient for calculaton of resonances of a junction, than another.

5 Example

Consider an example of a network, studied by modified analytic technique in [14]. Now we demonstrate the direct computational technique based on the same example. This permits to estimate the efficiency of the direct computing and to confirm the validity of the modified analytic perturbation technique, see [19].

Let Ω be a simplest asymmetric T-junction of three straight leads width $\pi/2$ attached to the quantum well - the square Ω_{int} on ξ -plane : $0 < \xi_1 < \pi$, $0 < \xi_2 < \pi$. Assume that the first wire $\omega_1 = \{-\infty < \xi_1 < 0, \pi/2 < \xi_2 < \pi\}$ is attached orthogonally to the left side of $\partial\Omega$ on $\Gamma_1 = \{\xi_1 = 0, \pi/2 < \xi_2 < \pi\}$, the second wire $\omega_2 = \{0 < \xi_1 < \pi/2, \pi < \xi_2 < \infty\}$ is attached in the middle of the upper side, and the third wire $\omega_3 = \{\pi < \xi_1 < \infty, 0 < \xi_2 < \pi\}$ is attached to the middle of the right side of Ω_{int} . On the constructed quantum network

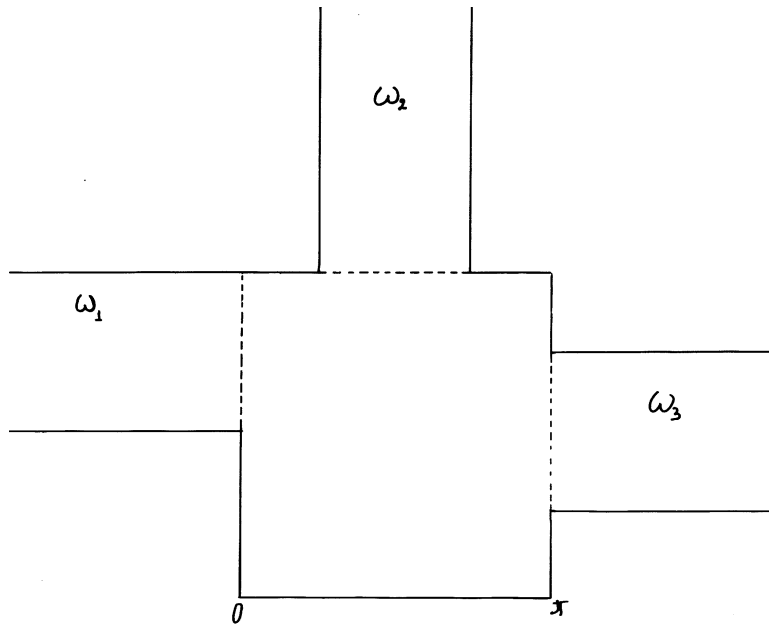


Figure 3: Simplest asymmetric T-junction

$\Omega = \Omega_{int} \cup \omega_1 \cup \omega_2 \cup \omega_3$ consider the scattering problem for Laplacian with homogeneous Dirichlet boundary condition at the boundary. The cross-section eigenfunctions in the first spectral channel in the wires $\omega_1, \omega_2, \omega_3$ are :

$$e^1 \Big|_{\Gamma_1} = \frac{2}{\sqrt{\pi}} \sin 2\xi_2, \quad e^2 \Big|_{\Gamma_2} = \frac{2}{\sqrt{\pi}} \cos 2\xi_1,$$

$$e^3 \Big|_{\Gamma_3} = \frac{2}{\sqrt{\pi}} \cos 2\xi_2$$

The Dirichlet Laplacian on Ω_{int} has on the first spectral band $\Delta_1 = [4, 16]$ the eigenvalues $\lambda_0 = 5, \lambda_1 = 8, \lambda_2 = 10$ and $\lambda_3 = 13$ with eigenfunctions $\Phi_0, \Phi_1, \Phi_2, \Phi_3$, $\Phi_0 = \frac{2}{\pi} \sin \xi_1 \sin 2\xi_2$. The boundary currents of Φ_0 are

$$\begin{aligned} \frac{\partial \Phi_0}{\partial n} \Big|_{\Gamma_1} &= -\frac{2}{\pi} \sin 2\xi_2, \quad \frac{\partial \Phi_0}{\partial n} \Big|_{\Gamma_2} = -\frac{4}{\pi} \sin \xi_1, \\ \frac{\partial \Phi_0}{\partial n} \Big|_{\Gamma_3} &= \frac{2}{\pi} \sin 2\xi_2. \end{aligned}$$

Assume that the Fermi level of the material is situated between the first and the second thresholds of the network $4 < E_F < 16$ close to the eigenvalue $\lambda_0 = 5 \text{ cm}^{-2}$, $\lambda^F = 4.33 \text{ cm}^{-2}$. The electrons are supplied to the network in the first spectral band from the second wire across the bottom section Γ_2 and exit across Γ_1, Γ_3 . Due to orthogonality of the cross-section eigenfunction of the open spectral channel to the boundary currents of the eigenfunctions Φ'_0, Φ'_3 the corresponding modes are not excited. An essential link to the closed spectral channels is supplied only by Φ_0 , the contribution from other eigenfunctions either vanish or are suppressed due to the factors $(\lambda_0 - \lambda_s)$ in the denominator. Then the normalized vector of the boundary current is $e_0 = (-0.8, 0.6, 0)$, and the boundary conditions at the junction for low temperatures are represented by the formulae (27) with $P_0 = e_0 \langle e_0$, which is different from the condition for a symmetric junction suggested in [16] for symmetric T-junction. For the higher temperatures the boundary condition is energy dependent and can be represented in form (44), with the approximate scattering matrix

$$S_{appr}(p) = \frac{i\sqrt{\lambda - 4}P_+ - 0.15\frac{P_0}{\lambda - 4.33}}{i\sqrt{\lambda - 4}P_+ + 0.15\frac{P_0}{\lambda - 4.33}}, \quad (43)$$

and $P_0 = e_0 \langle e_0$.

It is interesting to notice, that accurate computing done as described above, section 4, gives the same results for the scattering matrix, as a crude approximate calculation done in [14], on the first step of the analytic perturbation procedure. This confirms the validity our approach to the calculation of transport properties of the junction .

6 Manipulation of the transmission across the junction and trapped modes

The explicit expression for the scattering matrix of the junction may be derived from a solvable model of the junction in form of a quantum graph, with a one-dimensional Schrödinger equation $\psi'' + p^2\psi = 0$, with $p^2 = \lambda - 4$, and the boundary condition at the junction, defined such that the scattering matrix of the graph coincides with the scattering matrix if the junction

$$ip[I - S_{appr}(\lambda)]\vec{\psi} = [I + S_{appr}(\lambda)]\vec{\psi}'. \quad (44)$$

Here $\vec{\psi}, \vec{\psi}'$ are vectors of the boundary values of ψ at the vertex. The polar terms in the numerator and in the denominator of (43) can be represented via the relevant one-dimensional orthogonal projection $P_0 := \vec{e}_0 \langle \vec{e}_0$ with $\vec{e}_0 := (e_0^1, e_0^2, e_0^3) = \|\vec{\phi}_0\|^{-1} \vec{\phi}_0 := \alpha^{-1} \vec{\phi}_0$. Then $\vec{\phi}_0 \langle \vec{\phi}_0 = \alpha^2 P_0$. Denoting by P_0^\perp the complementary projection $I - P_0$ in $L_2(\Gamma)$, we

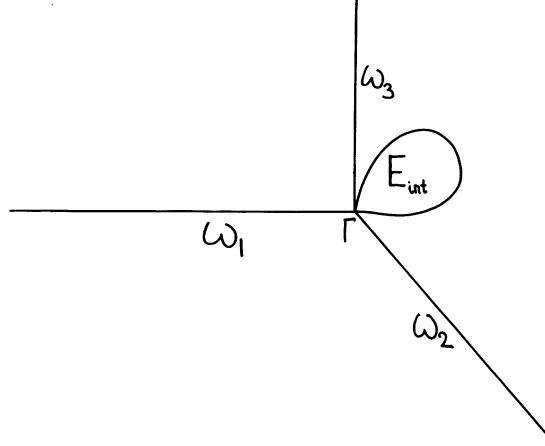


Figure 4: 1-d model of T-junction

obtain

$$\begin{aligned} S_{approx}(\lambda) &= P_0^\perp + \left[\frac{ip(\lambda - \lambda_0) - \alpha^2}{ip(\lambda - \lambda_0) + \alpha^2} \right] P_0 \\ &\equiv P_0^\perp + \Theta(\lambda) P_0. \end{aligned} \quad (45)$$

The factor

$$\Theta = \frac{ip - \frac{\alpha^2}{\lambda - \lambda_0}}{ip + \frac{\alpha^2}{\lambda - \lambda_0}}$$

is close to -1 on the essential spectral interval Δ_T . Then, in first approximation, the energy-dependent boundary condition (44) is reduced on Δ_T to $iP_0^\perp \psi - P_0 \psi' \approx 0$, or, due to orthogonality of P_0, P_0^\perp , to $P_0^\perp \vec{\psi} \approx 0$; $P_0 \vec{\psi}' \approx 0$, see [?]. This condition correlates with some rescription of Datta condition,[16]. But our analysis in [14] reveals the meaning of the projection P_0 : it coincides with the projection onto the one-dimensional subspace defined by the vector ϕ_0 of boundary values of the normal derivatives of the resonance eigenfunction, projected onto E_+ .

It is clear that the shape of the vertex domain and the coefficient $a(x, y)$ on it can be chosen, based on the formula (43) to optimize the transport properties of the junction.

The approximate formula (43) may be also used to calculate approximately the resonances- the zeros of the scattering matrix. Once the zero $\lambda_s = p_s^2$, $\Im p_s < 0$ is

found, $S(\lambda_s)e_s = 0$, we are able to obtain the corresponding solution of the stationary wave equation with the no-square integrable component in ω :

$$\Psi(p_s) = e^{iK+x}e_s, \quad e_s \in E_+.$$

Then the corresponding mode of the non-stationary wave equation is

$$e^{-\tau(p_s)t}e^{iK+x}e_s, \quad S(p_s)e_s = 0$$

where $i\tau(i\tau + \nu) + p^2$, $\omega(p) = i\nu/2 \pm \sqrt{-\nu^2/4 + p^2}$. If $\nu \ll p_s$ we have $\sqrt{-\nu^2/4 + p_s^2} \approx p_s - \nu^2/8p_s$. Then for $\nu \ll |p_s|$ we have the following expression on the leads ω for the exponentially dissipating on the junction *trapped mode* associated with the resonance p_s . The corresponding formal solution of the homogeneous stationary equation tends $t \rightarrow \infty$ on the wires. It can be interpreted in terms of Lax-Phillips scattering for corresponding solvable model.

7 Acknowledgement

The authors are grateful to Professor V. M. Adamyan for a hint concerning the elegant formula for the scattering matrix in terms of the ND - map. We also express our gratitude to Doctor L. Parnovskii for precious bibliographic data.

References

- [1] A. Chaplik *Possible crystallization of charge carriers in low-density inversion layers* Sov. Phys.JETP, **32** (1972), pp 395-398.
- [2] M. Dyakonov, M. Shur *Shallow water analogy for a ballistic field effect transistor: new mechanism of plasma wave generation by dc current* Phys. Rev. Letters, **71**, 15 Oct. 1993, pp 2465-2468
- [3] V. Ryzhii, I. Khmyrova, A. Satou *Plasma mechanism of Terahertz photomixing in high-electron mobility transistor under interband photoexcitation* Journ. Appl. Physics., **92**,10 (2002)
- [4] V. Ryzhii, A. Satou, M.S. Shur *Admittance of a slot diode with a two-dimensional electron channel* In: Journal of Applied Physics **93**, 12, (June 15 2003) pp 10041-10045
- [5] T. Otsuji, M. Hanabe, J. Shigenobu, S. Takahashi, E. Sano *A Nobel Terahertz Plasma-Wave Potomixer with Resonant -Cavity Enhanced Structure* Digest of the technical papers of the 12th IEEE Int. Conf. Terahertz. Electron., Sep. 2004
- [6] W. Knap, F. Teppe, Y. Mezani, N. Dyakonova, J. Lusakovski, F. Boeuf, T. Shotnicki, D. Maude, S. Rumyantsev, M. Shur *Plasma wave detection of subterahertz and terahertz radiation by silicon field-effect transistors* Appl. Phys. Rev., **85**, 4, JUL. 2004, pp 675-677.

- [7] A. Mikhailova, B. Pavlov, V.Ryzhii *Dirichlet-to-Neumann techniques for plasma waves in a slot-diod*, in: *Operator Theory: Advances and Applications*, Vol. 174, 59-85 (2007), Birkhäuser, Basel, Switzerland.
- [8] D. Pierotti Uniqueness and trapped modes in the linear problem of the steady flow over a submerged hollow In: *Wave Motion*, **43** (2006),pp 222-231.
- [9] R. Mittra, S. Lee *Analytical techniques in the theory of guided waves* The Macmillan Company, NY, Collier-Macmillan Limited, London, 1971.
- [10] R. Courant, . Hilbert, *Methods of mathematical physics. Vol. II. Partial differential equations*. Reprint of the 1962 original. Wiley Classics Library. A Wiley-Interscience Publication. John Wiley & Sons, Inc., New York, 1989. xxii+830 pp.
- [11] J. Sylvester, G. Uhlmann The Dirichlet to Neumann map and applications. In: *Proceedings of the Conference "Inverse problems in partial differential equations (Arcata, 1989)"*, SIAM, Philadelphia, 101 (1990)
- [12] B. Pavlov. S-Matrix and Dirichlet-to-Neumann Operators In: *Encyclopedia of Scattering*, ed. R. Pike, P. Sabatier, Academic Press, Harcourt Science and Tech. Company (2001) pp 1678-1688
- [13] N. Bagraev, A. Mikhailova, B. S. Pavlov, L. V. Prokhorov, and A. Yafyasov. *Parameter regime of a resonance quantum switch* *Phys. Rev. B*, 71:165308, 2005.
- [14] M. Harmer, B. Pavlov, A. Yafyasov *Boundary condition at the junction*, in: *Journal of Computational Electronics*, DOI 10.1007/s10825-006-0085-7
- [15] A. Mikhailova, B. Pavlov, L. Prokhorov *Modelling of quantum networks* arXiv math-ph/031238, 2004, 69 p.
- [16] S. Datta. *Electronic Transport in Mesoscopic systems*. Cambridge University Press, Cambridge, 1995.
- [17] J. Splettstoesser, M. Governale, and U. Zülicke. Persistent current in ballistic mesoscopic rings with Rashba spin-orbit coupling. *Phys. Rev. B*, 68:165341, 2003.
- [18] I. A. Shelykh, N. G. Galkin, and N. T. Bagraev. Quantum splitter controlled by Rashba spin-orbit coupling. *Phys. Rev. B* **72**,235316 (2005)
- [19] V. Adamyan, B. Pavlov, A. Yafyasov *Modified Krein formula and analytic perturbation procedure for scattering on arbitrary junction* Preprint of the International Newton Institute, NI07016, 18th April 2007, 30 p.
- [20] B.Pavlov *A star-graph model via operator extension* *Mathematical Proceedings of the Cambridge Philosophical Society*, Volume 142, Issue 02, March 2007, pp 365-384 doi: 10.1017/S0305004106009820, Published online by Cambridge University Press 10 Apr 2007.

- [21] I. S. Gohberg and E. I. Sigal. *Operator extension of the theorem about logarithmic residue and Rouché theorem* Mat. Sbornik. **84**, 607 (1971)
- [22] A. Mikhailova, B. Pavlov, L. Prokhorov *Intermediate Hamiltonian of a quantum network via Glazman splitting and analytic re-normalization procedure* 66 p. Accepted by Mathematische Nachrichten.
- [23] M. Levitin *A simple calculation of eigenvalues and resonances in domains with regular ends* arXiv:math.SP/0611237 v1 8 Nov 2006, 28 p.
- [24] Y. Colin de Verdière, Y.: *Pseudo-Laplacians II* Ann. Inst. Fourier **33** (1983) pp 87-113.
- [25] H. Donnely *Eigenvalue estimates for certain noncompact manifolds* Mich. Math. J. **31** (1984) pp 349-357.
- [26] L. Guillopé, *Théorie spectrale de quelques variétés à bouts* Ann. Sci. École Norm. Sup. (4) **22**, N. 1, 137-160 (1989)
- [27] W. Müller *Manifolds with cusps of rank one* Lect. Notes in Math., **1244** Springer-Verlag (1987)
- [28] L. Parnowski *Spectral asymptotics of the Laplace operator on manifolds with cylindrical ends* Int. J. Math., 6(1995), No. 6, 911-920.
- [29] L. Schwartz *Théorie des Distributions* Hermann, Paris, 1957.
- [30] A.A. Samarskij *Teoriya raznostnyh schem* In Russian, Nauka, Moskow 1977, 656 p. German translation: A.A.Samarskij *Theorie der Differenzverfahren* In: Mathematik und ihre Anwendungen in Physik und Technik, **40**, Academic Verlagsgesellschaft Geest&Portig, Leipzig 1984, 356 p.
- [31] J.H. Wilkinson, C. Reinsch (eds.) *Handbook for Automatic Computation. Volume 2: Linear Algebra* Berlin-Heidelberg-New-York, (1971), 439 p.
- [32] V. Adamyan, H. Langer, R. Mennicken *Spectral decomposition of selfadjoint block operator matrices with unbounded entries* Mathematische Nachrichten **178** (1996) pp 43-80