Quantum Domain as a triadic relay

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Abstract

For a solvable model of triadic relay the magnitude of the govering constant electric field is specified such that the manipulation of the quantum current is possible via the change of the direction of the field in a plane parallel to the plane of the relay.

1 Introduction: low-dimensional structures and hybrid Schrödinger operators

In our previous papres [1], [2], [3] we considered mathematical models for quantum electronic devices designed to manipulate the quantum current in physical networks construted of quantum wires and quantum domains on the interface of an electrolyte and a narrow-gap semiconductor. The wires are created usually by itching as a narrow channels where the moleculae of the electrolyte form the conducting chain. Quantum domains may be formed on the surface of the semiconductor by epitaxy. Due to the narrow-gap property ([5],[4]) the effective mass m_e of electrons in the semiconductor is small compared with conventional electron's mass, $\frac{m_e}{m_0} \approx 0.01$, and hence the De-Broghlie wave-length Λ calculated from the effective Scrödinger equation

$$-\frac{\hbar^2}{2m_e}\Delta\Psi + V\Psi = E_g\Psi$$

at the Fermi level E_g may be large if compared with the width of the wires or the thickness of the domain (approximately $100 \div 200 \mathring{A}$)). This may be illustrated by the following Table (see [5],Section 3) and ([4]):

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Semiconductor	E_g (300 K) eV	$\frac{m_e^*}{m_0}$	$\frac{m_p^*}{m_0}$	ε_{sc}	Λ (300 K) Å	Λ (77 K) Å
$GaAs$	1.430	0.070	0.40	12.5	290	580
$InAs$	0.360	0.022	0.40	15.0	515	1020
$Cd_xHg_{1-x}Te$						
$x = 0.20$	0.150	0.0130	0.45	17.0	670	1320
$x = 0.25$	0.220	0.0165	0.45	16.4	590	1160
$x = 0.27$	0.250	0.0180	0.45	16.2	570	1125
$x = 0.28$	0.260	0.0190	0.45	16.1	550	1085
$x = 0.29$	0.275	0.0200	0.45	16.0	540	1065
$x = 0.30$	0.290	0.0210	0.45	16.0	525	1035
$x = 0.31$	0.300	0.0220	0.45	15.9	515	1015
$x = 0.32$	0.315	0.0230	0.45	15.8	500	985
$x = 0.44$	0.510	0.0550	0.45	15.2	325	640
$HgTe$	-0.117	0.012	0.50	21.0	700	1380
$Zn_{0.15}Hg_{0.85}Te$[1]	0.190	0.015	0.45	17.0	620	1220

This means that the wires are effectively one-dimensional and the domains are two-dimentional objects, so that the physical network of wires and domains becomes a *hybrid system* and the effective Schrödinger operator becomes effectively a coupling of ordinary differential operators on the wires and partial differential operators on the domains, connected by proper boundary conditions at the points of contact.In actual paper we continue investigation of the simplest example of a network designed for implementation of operations of triadic logic .

Basing on mentioned above low-dimensional properties os narrow-gap semiconductors and following general ideas described in [2] we construct in actual paper a solvable model of a triadic relay as a dwo-dimensional circular domain Ω with a few (eventually $N = 4$) one-dimensional wires Γ_s attached to it. The corresponding hybrid Hamiltonian is formed as a common selfadjoint extension of a couple of Schrödinger operators acting in the orthogonal sum $\mathcal{H} = \oplus \sum_s L_2(\Gamma_s) \oplus L_2(\Omega)$ of Hilbert spaces of all square-integrable functions on the wires and on the domain. At the points of contact of the domain and the wires we connect the functions from the domain of the components of the Hamiltonian via special boundary conditions which may characterize the strength of the contact between the wires and the domain. To avoid awkward notations we assume for the beginning that the dimensionless coordinates are used, so that the underlying differential equations look like

$$-\frac{d^2\Psi}{dx^2} = \lambda\Psi \tag{1}$$

on the wires and

$$-\Delta\Psi + V\Psi = \lambda\Psi \tag{2}$$

[1] In series of triple compounds A_2B_6, this material is more prospective in technology, as its properties are considerably more stable in comparison with $Cd_xHg_{1-x}Te$.

[2] The above mentioned "narrow-gap properties" imply important physical phenomena such as high-temperature quantum behaviour,in particular the possibility of simulated Peirls transition,which may be also used for manipulating quantum current, ([4])

on the domain. The exact potential for manipulation the transmission across the domain will be chosen later. The simpliest but still convenient option is a linear potential of some constant electric field intensity ε directed along the vector $\mathbf{e}$:

$$V(\mathbf{X}) = \langle \mathbf{x}, \mathbf{e} \rangle \ \varepsilon$$

$$\nabla V = \varepsilon \ \mathbf{e}.$$

The intensity ε will be defined from the conditions for the transmission coefficients, see section 3 below.

To introduce the boundary conditions for our model at the points of contact we begin with operators defined on the wires $\Gamma_i \quad 1 = 1, 2, 3, 4$ and on the domain Ω with homogenious Neuman boundary conditions:

$$\frac{du_s}{dx}|_{x=0} = 0$$

$$\frac{\partial u_0}{\partial n}|_{\partial\Omega} = 0.$$

The third boundary condition

$$\frac{\partial u_0}{\partial n} - \sigma u|_{\partial\Omega} = 0$$

at the boundary $\partial\Omega$ of the domain may give even more interesting option permitting modelling a large scale of boundary behaviour including the loose ($\gamma = 0$) and hard ($\gamma = \infty$) joining of the domain to the environment. The magnitude of σ might be interpreted as a common characteristics of the potential barrier on the border of the domain and the density of the electrical double layer on the interface of the domain and environment, and may formally represented as an additional potential.Then the corresponding Scrödinger equation may be written in form

$$-\Delta\Psi + [V_{bulk} + V_g + \sigma'\delta(dist(x, \partial\Omega))]\Psi = \lambda\Psi$$

where V_{bulk} is a step-vise function : $V_{bulk} = V_0$ inside the domain and $V_{bulk} = V_1 >> 1$ outside of it, V_g is the *govering* potential of a constant electric field $V_g = \langle x, \mathbf{e} \rangle \varepsilon$, used for manipulating the electron's current across the domain, and the singular term $\sigma'\delta$ attached to the boundary corresponds to an additional polarization of the electrolyte near the boundary of the domain. The straightforward integration by parts shows that the singular term gives the boundary condition

$$[\frac{\partial u}{\partial n}] - \sigma' u|_{\partial\Omega} = 0$$

For high barrier $V_1 >> E_g$ we may assume that for electrons at Fermi level at low temperatures $\frac{\partial u}{\partial n_e} \cong -(V_1 - E_g)u|_{\partial\Omega}$ which gives due to continuity of u at the boundary

$$\frac{\partial u}{\partial n} + (\sigma' + V_1 - E_g)u|_{\partial\Omega} = 0$$

If we denote $\sigma' + V_1 - E_g$ by σ then the homogeneous Neumann boundary condition corresponds to the special case $\sigma' + V_1 - E_g = 0$. In what follows we assume that this is exactly the case, though the analysis based on the general third boundary condition may add in fact some minor technical complications.

2 Solvable model of a triadic relay

Following ideas of our previous paper we construct the solvable model of a triadic relay as a "mixing" selfadjoint extension of the underlying operators

$$L = -\Delta + V \text{ in } L_2(\Omega)$$

with Neumann boundary condition at the boundary and

$$l_s = -\frac{d^2}{dx^2} \text{ in } L_2(\Gamma_s)$$

on the wires $\Gamma_s,\ s = 1, 2, \ldots N$ with Neumann boundary condition at the origin, reduced preliminary onto the linear set of elements from the domains vanishing near the points of contact.

To describe the extension procedure we need the deficiency elements and the boundary conditions. Consider the selfadjoint operator $L = -\Delta + V$ in $L_2(\Omega)$ with any continuous potential V including both bulk and govering component, and homogeneous Neumann boundary condition

$$\frac{\partial u}{\partial n}|_{\partial\Omega} = 0 \tag{3}$$

on the boundary. The corresponding Green function $G_\lambda(x, y)$ is a singular solution of the homogeneous equation

$$-\Delta G + VG = \lambda G \tag{4}$$

with a special behaviour at the inner pole y :

$$G_\lambda(x,\, y) = \frac{1}{2\pi} \log \frac{1}{|x-y|} + O(1)$$

when $|x - y| \to 0$ and satisfying the homogeneous Neumann boundary conditions.For zero-potential the main singular solution on the whole plane is just Hankel-function of the first kind $\frac{i}{4}H_0^1(\sqrt{\lambda}|x-y|)$ and the Green-function for zero-potential is represented in form of a sum of the corresponding main singular solution and a regular solution of the corresponding homogeneous equation

$$G_\lambda^0(x,\, y) = \frac{i}{4}H_0^1(\sqrt{\lambda}|x-y|) + g_\lambda(x,\, y), \tag{5}$$

$$-\Delta g = \lambda g,$$

$$\frac{\partial g}{\partial n}|_{\partial\Omega} + \frac{i}{4}\frac{\partial H_0^1(\sqrt{\lambda}|x-y|)}{\partial n}|_{\partial\Omega} = 0$$

The Green-function of the Schrödinger equation (4) may be found as a solution of the Lippman-Schvinger equation

$$G_\lambda(x,\, y) = G_\lambda^0(x,\, y) + \int_\Omega G_\lambda^0(x,\, s)V(s)G_\lambda^0(s,\, y)ds^2 \tag{6}$$

from which one may deduce easily that it has the same singularity at the pole as the Green-function of the Laplace equation.If the boundary $\partial\Omega$ in smooth, then one may

derive that the Green function of Laplace equation has the logarithmic singularity at the boundary pole $y \in \partial\Omega$

$$G_\lambda(x,\, y) \approx \frac{1}{\pi} \log \frac{1}{|x-y|},\ x \to y. \tag{7}$$

Then from the above Lippman-Schwinger equation we may obtain that the Green-function of the Schrödinger equation has the same singularity at the boundary points described by (7), which implies the square integrability of the Green-function for any position of the pole in Ω. Note that the gradients of Green-functions $G_\lambda(x,\, a_s),\ s = 1,\, 2,\, \ldots N$ are not square-integrable, which means, that the deficiency indices of the operator L reduced $L \to L_0$ onto the linear set of all elements from the domain D_L of L vanishing near the points $a_1,\, a_2,\, a_3,\, \ldots a_N$ are equal $(N,\, N)$, and the Green-functions $G_\lambda(x,\, a_s),\ s = 1,\, 2,\, \ldots N$ play the role of deficiency elements.

Planning to use the symplectic version of the operator extension procedure, see [15], [13] we introduce the asymptotis boundary values:*singular amplitudes* $A_s(u)$ and the *regularized values* $B_s(u)$ for elements u of the domain of the adjoint operator L_0^+ at the points a_s. We assume now that the nonperturbed Schrödinger operator $L + I$ on the domain Ω with Neumann boundary condition is definitely positive $L + I > 0$. Then its resolvent $[L+1]^{-1}$ is a bounded integral operator with the kernel $G_{-1}(x, y)$. We use this kernel as an etalon of the growing rate for elements of the domain of adjoint operator at the poles:

$$u(x) = A_s^1 G_{-1}(x, a_s) + B_s^1 + o(1),\ x \to a_s. \tag{8}$$

The next statement shows that both A_s^1, B_s^1 exist for deficiency elements $e_{\bar\lambda} = G_\lambda(x, a_s)$.

Lemma 2.1 *For any regular point λ from the complement of the spectrum $\sigma(L)$ of the operator L and any $a \in \{a_s\}_{s=1}^N$ the following representation is true:*

$$G_\lambda(x, a) = G_{-1}(x, a) + (\lambda + 1) G_{-1}^+ G_\lambda(x, a),$$

where the second addend $(\lambda+1)G_{-1}^+ G_\lambda(x,a) \equiv g_\lambda(x,a)$ is a continuous function of x and the spectral series of it on eigenfunctions φ_l of the operator L,

$$L\varphi_l = \lambda_l \varphi_l,$$

is absolutely and uniformly convergent in Ω. The separation of the singularity at each eigenvalue λ_0 is possible:

$$g_\lambda(x,a) = (\lambda+1) \sum_l \frac{\varphi_l(x)\varphi_l(a)}{(\lambda_l+1)(\lambda_l - \lambda)} =$$

$$\frac{\varphi_0(x)\varphi_0(a)}{\lambda_0 - \lambda} + g_\lambda^0(x,a) \tag{9}$$

with uniformly and absolutely convergent series for $g_\lambda^0(x,a)$ in a neighbourhood of λ_0.

Proof of the $3-d$-version of this statement is given in ([2]). We sketch it here just for the convenience of the reader.

The analysis of the Lippman-Schwinger equation (6) shows that the Green function $G_\lambda(x,y)$ of the operator L admitts a representation in form (7) which implies that the positive integral operator $G_{-1}*G_{-1}$ has a continuous kernel on the closed domain $\Omega = \overline{\Omega}$. Then using smothness of the normalized eigenfunctions

$$|\varphi_s|_{\mathrm{Lip}_{\frac{1}{2}}} \leq \mathbf{C}|\varphi_s|_{W_2^2(\Omega)} \leq$$

$$\leq (\sup_\Omega |V(x)| + |\lambda_s|)$$

and the classical Mercer theorem we may check that the spectral series for it's kernel

$$(\lambda+1)G_{-1}*G_{-1}(x,y) = (\lambda+1)\sum_l \frac{\varphi_l(x)\varphi_l(y)}{(\lambda_l+1)^2}$$

is converging absolutely and uniformly in Ω. From the last statement we derive that the spectral series for the kernel on the diagonal $x = y$ is also convergent absolutely and uniformly. Then using the Cauchy estimate for the remainder of the spectral series for the kernel

$$G_{-1}*G_\lambda(x,y) = \sum_l \frac{\varphi_l(x)\varphi_l(y)}{(\lambda_l+1)(\lambda_l-\lambda)}$$

on the closed domain $x,\, y \in \overline{\Omega}$ and λ sitting on each compact subset of the complement of the spectrum $\sigma(L)$, we may derive that the spectral series for the iterared resolvent kernel $G_{-1}*G_\lambda(x,y)$ is convergent absolutely and uniformly. Together with the continuity of eigenfunctions this implies the continuity of $G_{-1}*G_\lambda(x,y)$ on the complement of the spectrum and the continuity of the difference

$$g_\lambda^0(x,y) \equiv (\lambda+1)G_{-1}*G_\lambda(x,y) - \frac{\varphi_0(x)\varphi_0(y)}{\lambda_0-\lambda} =$$

$$\sum_{l\neq 0} \frac{(\lambda+1)\varphi_l(x)\varphi_l(y)}{(\lambda_l+1)(\lambda_l-\lambda)} - \frac{\varphi_0(x)\varphi_0(y)}{\lambda_0+1}$$

in some neighbourhood of the eigenvalue λ_0.

□

We shall follow the constructive Krein approach to the description of selfadjoint extension of the reduced operator, both in $L_2(\Omega)$ and in extended spaces, connecting directly the resolvents of different selfadjoint extensions by explicite formulae. To derive the corresponding Krein formulae we need a special representation for elements of the the domain of the adjoint operator L_0^+.

Denote by $N_{\pm i}$ the deficiengy subspaces of the restricted symmetric operator L_0. Consider an orthogonal and normalized basis $e_i^s \in N_i$ and the corresponding basis $e_{-i}^s = \dfrac{\mathcal{A}+iI}{\mathcal{A}-iI}$ in N_{-i}:

$$\mathcal{A}e_{\pm i}^s + (\pm i)e_{\pm i}^s = 0.$$

Basing on the statement of the preceeding Lemma we may introduce a special basis, see [15], in the direct sum of the deficiency subspaces N_i, N_{-i}, formed of linear combinations $W_\pm^s$ of the deficiency elements $e_{\pm i}^s$

$$W^s_+ = \frac{e^s_i + e^s_{-i}}{2} = \frac{\mathcal{A}}{\mathcal{A} - iI} e^s_i$$

$$W^s_- = \frac{e^s_i - e^s_{-i}}{2i} = \frac{I}{\mathcal{A} - iI} e^s_i$$

We see that

$$\mathcal{A}^+_0 W^s_+ = -W^s_-,$$
$$\mathcal{A}^+_0 W^s_- = W^s_+.$$

From the previous Lemma follows that the elements W^s_+ have singularities at the set $\{a_s\}$ but the elements W^s_- are continuous.

Consider the domain D^+_0 of the adjoint operator L^+_0. According to the classical formulae of von-Neumann operator extension theory, for densely defined operator L_0 the domain D^+_0 of adjoint operator may be represented in form of a direct sum $D_0 + N_i + N_{-i}$. Using the basis introduced above we define the symplectic coordinates $\xi^s_\pm$ for the element $u \in D^+_0$ as coefficients in the direct decomposition

$$u = u_0 + \sum_s \xi^s_+ W^s_+ + \sum_s \xi^s_- W^s_- = u_0 + \frac{L}{L - iI}\vec{\Xi}_+ + \frac{I}{L - iI}\vec{\Xi}_- \tag{10}$$

where $\vec{\Xi}_\pm = \sum \xi^s_\pm e^s_i \in N_i$ and the component of u from the domain D_0 of the restricted Hermitian operator L_0 is denoted by u_0. From the general scheme [15] we see that the boundary form of the adjoint operator $(L_0)^+$ may be represented as a *complex symplectic form* of variables $\xi^s_\pm$:

$$\mathcal{J}_L(u,v) := \langle L^+_0 u, v\rangle - \langle u, L^+_0 v\rangle =$$
$$= \langle \vec{\Xi}_-, \vec{\Xi}^v_+\rangle - \langle \vec{\Xi}^u_+, \vec{\Xi}^v_-\rangle =$$
$$= \sum_s \left[\xi^s_-(u)\overline{\xi}^s_+(v) - \xi^s_+(u)\overline{\xi}^s_-(v)\right] < e^s_i, e^s_i > . \tag{11}$$

The previous lemma implies existence of *regularized boundary values*

$$\lim_{x \to a_s} [G_\lambda(x, a_s) - \Re G_i(x, a_s)]$$

for each deficiency element $G_i(x, a_s)$ and hence for all linear combinations of them. In particular each element $u = u_0 + \sum_s A^+_s G_i(x, a_s) + \sum_s A^-_s G_{-i}(x, a_s)$ of the domain of the adjoint operator D^+_0 also has the regularized boundary values defined as

$$\lim_{x \to a_t} \left[u(x) - \sum_s A^s \Re G_i(x, a_s)\right] := B_t, \;\; A_s = A^+_s + A^-_s.$$

Together with *singular amplitudes* A_s they form another set of symplectic coordinates which may be also used to represent the boundary form of L^+_0 as a complex symplectic form

$$\mathcal{J}_L(u,v) = \langle L^+_0 u, v\rangle - \langle u, L^+_0 v\rangle =$$
$$\sum B^u_s \bar{A}^v_s - A^u_s \bar{B}^v_s := \langle \vec{B}^u, \vec{A}^v\rangle - \langle \vec{A}^u, \vec{B}^v\rangle \tag{12}$$

One can see that at the boundary points a_s of the domain Ω these boundary values are connected with commonly used, see [16], [15] asymptotic boundary values $\hat{A}_s$, $\hat{B}_s$ of u defined as coefficiens of the asymptotics at the point a_s:

$$u(x) \approx \frac{\hat{A}_s^u}{\pi} \log \frac{1}{|x - a_s|} + \hat{B}_s^u + o(1),$$

by some linear J-unitary transformation, which leaves the boundary form unchanged . In particular for single element $G_\lambda(x, a)$ we have , see [15] and also below (15), the following formula :

$$G_\lambda(x, a) = \Re G_i(x, a) + \frac{I}{L - iI} P_{N_i} \frac{I + \lambda L}{L - \lambda I} G_{-i}(x, a) + u_0,\ u_0 \in D_0,$$

hence

$$B = \langle \frac{I + \lambda L}{L - \lambda I} G_{-i}(x, a),\ G_{-i}(x, a) \rangle.$$

and $A = 1$ for onedimensional deficiency subspace if the basis $G_{-i}(x, a)$ is used . The asymptotic values $\hat{A}_s$, $\hat{B}_s$ also may be used as symplectic variables to write down the boundary form in symplectic fashion. Really from the asymptotics of the Green-function we see that

$$\Re G_i(x, a) = \frac{\hat{A}_s^i}{\pi} \log \frac{1}{|x - a|} + C_i + o(1),$$

which means that for $\hat{A}_s^G = 1, C_i = \bar{C}_i$. Comparing asymptotic values of $G_\lambda(x, a)$ we see that

$$\hat{A}^G = A^G = 1,\ \hat{B}^G = B^G - C_i,$$

hence for deficiency elements $u = A_+ G_\lambda(x, a) + A_- G_{\bar{\lambda}}(x, a)$ the asymptotic boundary values $\hat{A}, \hat{B}$ and A, B are connected by the transformation

$$\begin{pmatrix} \hat{A} \\ \hat{B} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -C_i & 0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

which does not change the values of the boundary form (is $\mathcal{J}$-unitary):

$$\hat{B}^u \bar{\hat{A}}^v - \hat{A}^u \bar{\hat{B}}^v = B^u \bar{A}^v - A_u \bar{B}^v,$$

hence these two sets of symplectic variables are equivalent. But still the spectral meaning of the symplectic variables B_s is more transparent, see below. For this reason we use further exclusively the variables A_s, B_s.

Using the above representation for elements of the domain of adjoint operator (32) we may derive the explicite expression for the regularized boundary values of elements of deficiency subspace $u = \sum_{s=1}^N A_s G_\lambda(x,\ a_s)$. They serve solution of the adjoint homogeneous equation

$$\mathcal{A}_0^+ u = \lambda u. \tag{13}$$

It follows from the Lemma 1 that the singular amplitudes A_s^u of u coincide with A_s. The next step is to express the regularized boundary values B_s in terms of singular

amplitudes for any solutions u of the *adjoint homogeneous equation* (13). The operator Q which transforms the vector of singular amplitudes $\vec{A}$ into the vector of corresponding regularized boundary values $\vec{B}$ for the solutions of (13) is a simplest analog of so-called *Dirichlet to Neumann map* for elliptic partial differential eqations and at the same time it is a multidimensional version of Titchmarsh-Weyl function. In our scheme it appeares in form of Krein's Q-function, see [17]. It depends on λ and this dependence actually contains all essential spectral information of the nonperturbed operator $\mathcal{A}$.

To recover this information note first that the deficiency element $e_{\overline{\lambda}}$ for the spectral point $\overline{\lambda}$ serves the solution of the adjoint equation $(L_0^+ - \lambda)e_{\overline{\lambda}} = 0$ and may be expressed through the the deficiency element e_i for the spectral point i as

$$e_{\bar{\lambda}} = \frac{L + iI}{L - \lambda I} e_i.$$

One can see from it that

$$e_{\bar{\lambda}} = \frac{L + iI}{L - \lambda I} e_i = G_\lambda^L(x, a_s)$$

and

$$G_\lambda^L(x, a_s) - \Re G^L(x, a_s, i) = \frac{L + iI}{L - \lambda I} e_i^s - \frac{L}{L^2 + 1}(L + iI)e_i^s.$$

Then denoting $\delta(x - a^s)$ by δ^s we obtain:

$$\frac{I}{L - \lambda I}\delta^s - \frac{L}{L^2 + 1}\delta^s = \frac{1}{L - iI}\frac{1 + \lambda L}{L - \lambda I}\frac{1}{\mathcal{A} + iI}\delta^s.$$

One can easily see from the Lemma above that $\dfrac{I}{\mathcal{A} - \lambda I}\delta^s - \dfrac{L}{L^2 + 1}\delta^s$ is a continuous function of x near the point a_s and the limit of it :

$$\lim_{x \to a_s} [G_\lambda(x, a_s) - \Re G_i(x, a_s)] = \langle \frac{I + \lambda L}{L - \lambda I} G_i(a_s), G_i(a_s) \rangle := g^s(\lambda) \tag{14}$$

is just the regularized boundary value of $G_\lambda^L(x, a_s)$ at the point a_s. In particular for the sum of deficiency elements

$$u = \sum_s A_s G_\lambda(x, a_s)$$

we have the following asymptotics $x \to a_s$:

$$u = A_s \Re G_i(x, a_s) + g^s(\lambda) A_s + \sum_{t \neq s} A_t G_\lambda(a_s, a_t) + o(1). \tag{15}$$

where $A_s,\ B_s = g^s(\lambda)A_s + \sum_{t \neq s} A_t G_\lambda(a_s, a_t)$ define the symplectic variables of the element u.

Summarizing the calculations we have done deriving the last formula (15) we may formulate the following useful statement:

Lemma 2.2 *The singular amplitudes*

$$\vec{A}_+ = \begin{pmatrix} A_1 \\ A_2 \\ . \\ . \\ A_N \end{pmatrix}$$

and the regularized boundary values

$$\vec{B} = \begin{pmatrix} B_1 \\ B_2 \\ . \\ . \\ B_N \end{pmatrix}$$

of solutions of the homogeneous equation $L_0^+ u = \lambda u$ *are connected by the formula:*

$$\vec{B}^u = Q\vec{A}^u,$$

where

$$Q(\lambda) = \begin{pmatrix} g^1(\lambda) & G_\lambda(a_1,a_2) & .. & ... & G_\lambda(a_1,a_N) \\ G_\lambda(a_2,a_1) & g^2(\lambda) & .. & ... & G_\lambda(a_2,a_N,\lambda) \\ .. & .. & g^3(\lambda) & ... & .. \\ .. & .. & .. & ... & .. \\ G_\lambda(a_N,a_1) & .. & .. & ... & g^N(\lambda) \end{pmatrix} \tag{16}$$

Near the simple eignvalue λ_0 *the* Q*-matrix may be decomposed as*

$$Q_{st}(\lambda) = \frac{\bar{\varphi}_0(a_s)\varphi_0(a_t)}{\lambda_0 - \lambda} + (K_0)_{st}(\lambda) \tag{17}$$

where K_0 *is an analytic matrix-function in a neighbourhood of* λ_0*:*

$$(K_0)_{st}(\lambda) = \begin{cases} \sum_l \frac{\lambda_l}{1+\lambda_l^2}|\varphi_l(a_s)|^2, & s = t, \\ \left[G_\lambda(x,y) - \frac{\bar{\varphi}_0(x)\varphi_0(y)}{\lambda_0-\lambda}\right]|_{x=a_s,\, y=a_t}, & s \neq t \end{cases}$$

Note that the last statement is just a version of the general formula connecting the boundary values of abstract Hermitian operators, and Q plays the role of Krein's Q-function.

We shall use the decomposition (17) below in section 3 when exploring the resonance conductance across the domain.

The practical construction of the selfadjoint extensions of operators in the domain may be based on the following statement:

Theorem 2.1 *The restriction of the operator*

$$L = -\Delta + V \to L_0$$

onto the class of all W_2^2*- smooth functions which satisfy homogeneous Neumann boundary conditions and vanish near the boundary points* a_s, $s = 1, 2, \ldots N$ *is a symmetric operator with deficiency indices equal (N,N). The corresponding deficiency elements are Green-functions* $G_\lambda(x,\, a_s)$*. The domain of adjoint operator* L_0^+ *consists of all locally* W_2^2*- functions* u *defined on* $\Omega \backslash \{a_1,\, a_2,\, \ldots N\}$ *which have the asymptotic boundary values - singular amplitudes and regularized boundary values at the boundary points* $\{a_1,\, a_2,\, \ldots N\} \in \partial\Omega$ *:*

$$u(x) \approx A_s^u \Re G_i(x, a_s) + B_s^u, \;\; s = 1, 2, \ldots N, \tag{18}$$

connected via Q-matrix: $\vec{B}^u = Q\vec{A}^u$. *The boundary form of the adjoint operator may be represented in terms of asymptotic boundary values as a complex symplectic form :*

$$\mathcal{J}_L(u,v) := < L_0 u, v > - < u, L_0 v >= \sum_{s=1}^{N} \left\{ B_s^u \bar{A}_s^v - A_s^u \bar{B}_s^v \right\} \tag{19}$$

All selfadjoint extensions of the operator L_0 *in* $L_2(\Omega)$ *are parametrized by Lagrangian planes* $\mathcal{L}$ *of the boundary form (20) in the complex* $2N$*-dimensional space of variables* $\vec{A}, \vec{B}$ *:*

$$\mathcal{J}_L(u,v) = 0, \ \textit{if} \ \left\{ \vec{A}^u, \vec{B}^u \right\}, \ \left\{ \vec{A}^v, \vec{B}^v \right\} \in \mathcal{L}.$$

Proof of this statement may be obtained as a corollary of preceeding statements, see also ([2]). We shall use it as a basics when calculating the resolvents of hybrid Hamiltonians.

Together with the operator L_0 in $L_2(\Omega)$ we consider also the ordinary differential operators $l_s = -\frac{d^2}{dx^2}$ on the wires in $L_2(\Gamma_s)$, $s = 1, 2, \dots N$. The restriction $l_{s,0}$ of them onto classes of all W_2^2-smooth functions on the wires vanishing at the origine $x_s = 0$ gives Hermitian operators with deficiency indices $(1,1)$, and adjoint operators $l_{s,0}^+$ with boundary forms represented in terms of boundary values $u_s(0)$, $u_s'(0)$ of elements from the corresponding domains D_s^+ . Denoting by l^+ the orthogonal sum $\oplus \sum_{s=1}^N l_{s,0}^+$ we may represent the boundary form of l^+ in $\oplus \sum_{s=1}^N L_2(\Gamma_s)$ on elements $\vec{u} = \{u_1, u_2 \dots u_N\}$, $\vec{v} = \{v_1, v_2, \dots v_N\}$ as

$$\mathcal{J}_l(\vec{u}, \vec{v}) = < l^+\vec{u}, \vec{v} > - < \vec{u}, l^+\vec{v} >= \sum_{s=1}^{N} \{ u_s' \bar{v}_s - u_s \bar{v}_s' \}. \tag{20}$$

We construct now the selfadjoint extensions of the total reduced operator $L_0 \oplus l_0$in $\oplus \sum_{s=1}^N L_2(\Gamma_s)$ basing on analysis of the boundary form of the corresponding adjoint operator $L_0^+ \oplus l_0^+$ on elements $\{u, \vec{u}\}, \{v, \vec{v}\}$

$$\mathcal{J}_{L_0^+ \oplus l_0^+} = \mathcal{J}_L(u, v) + \mathcal{J}_l(\vec{u}, \vec{v}) = \sum_{s=1}^{N} \left\{ B_s^u \bar{A}_s^v - A_s^u \bar{B}_s^v \right\} + \sum_{s=1}^{N} \{ u_s' \bar{v}_s - u_s \bar{v}_s' \}. \tag{21}$$

All selfadjoint extensions of $L_0 \oplus l_0$ may be parametrized by Lagrangian planes of the the form (21). Imposing the *special* boundary conditions at the boundary points of contact a_s, $s = 1, 2, ..N$:

$$\begin{pmatrix} A_s \\ u_s(0) \end{pmatrix} = \begin{pmatrix} 0 & \beta \\ \beta & 0 \end{pmatrix} \begin{pmatrix} B_s \\ u_s'(0) \end{pmatrix}, \ \ \beta > 0, \ \ s = 1, 2, ..N. \tag{22}$$

we obtain, after closure, the selfadjoint operator $\mathbf{L}_\beta$ in $L_2(\Omega) \oplus \sum_{s=1}^N L_2(\Gamma_s)$ which will serve, subject to proper choice of the field ε, a solvable Hamiltonian of the triadic relay. Similarly to our previous paper [2] we decribe the spectral properties of the hybrid Schrödinger operator $\mathbf{L}_\beta$ basing on Krein formula connecting the resolvents of the underlying operator $\mathbf{L}_\infty := L \oplus \sum_{s=1}^N l_s$ with the resolvent of $\mathbf{L}_\beta$.

We derive an explicit formula for the component of the resolvent kernel (Green function) $G_\lambda^\beta(x,y)$ of the operator $\mathbf{L}_\beta$ on the domain Ω and compelte formulae for

scattered waves of the operator - the eigenfunctions of ansolutely-continuous spectrum $\sigma(\mathbf{L}_\beta)$. Similarly to our previous paper ([2]) we consider the *generic case* when neither of eigenfunctions of the nonperturbed operator L in $L_2(\Omega)$ vanishes at all contact points $a_s,\ s = 1, 2, ...N$ simultaneously. In what follows we assume that the singular amplitudes $\vec{A} := \{A_1, A_2, ...A_N\}$ and regularized boundary values are elements of an auxilliary finite-dimensional Hilbert space E, $\dim E = N$. We call this space the *channel space*, having in mind the role it plays in scattering problem. In particular we use vectors combined of the values of the nonperturbed Green functions attached to the points $\{a_s\} : \{G_\lambda(x, a_s)\} \equiv \vec{G}_\lambda(x)$. We assume that the metric form of E is standard, for instance the dot product of two vectors above is given by the formula:

$$< \vec{A}, \vec{G}^{\beta,0}_\lambda(x) >= \sum_s \bar{A}_s G^{\beta,0}(x, a_s, \lambda)$$

The hybrid Hamioltonians are described by the following statement which is in fact a version of the corresponding $3-d$ statement proven in ([2]):

Theorem 2.2 *The component $G^\beta_\lambda(x, y)$ of the the resolvent kernel of the operator $\mathbf{L}_\beta$ on the domain, $x, y \in \Omega$, is represented in terms of Green function of the nonperturbed operator L the following way:*

$$G^\beta_\lambda(x, y) = G_\lambda(x, y) + < \overline{\vec{G}_\lambda(y)}, \left[\frac{1}{ik\beta^2} - Q\right]^{-1} \vec{G}_\lambda(x) >,\ k^2 = \lambda,\ \Im k \geq 0. \tag{23}$$

The spectrum $\sigma(\mathbf{L}_\beta)$ of the perturbed operator $\mathbf{L}_\beta$ consists of all singularities of the matrix

$$\left[\frac{1}{ik\beta^2} - Q\right]^{-1}$$

in the complex plane of the spectral parameter $\lambda = k^2$, where Q is the Krein's Q-matrix described above, see (16). In particular the absolutely continuous spectrum of $\mathbf{L}_\beta$ fills the positive half-axis $\lambda \geq 0$ with the constant multiplicity N. The eigenvalues $\lambda_r = k_r^2,\ \Im k_r > 0$ and the resonances $\lambda_r = k_r^2,\ \Im k_r < 0$ of the operator $\mathbf{L}_\beta$ are defined, counting multiplicity, respectively: by the poles of the matrix $\left[\frac{1}{ik\beta^2} - Q\right]^{-1}$ on the positive imaginary half-axis (for eigenvalues $\lambda = k^2 < 0$) or in lower half-plane $\Im k < 0$ (for resonances). They may be found as roots of the corresponding dispersion equation in upper $\Im k > 0$ and lower $\Im k < 0$ half-planes (physical and nonphysical sheets) respectively:

$$det\left[\frac{1}{ik\beta^2} - Q\right] = 0. \tag{24}$$

The eigenfunctions of the absolutely- continuous spectrum of the operator $\mathcal{L}_{\beta,0}$ are presented by the scattered waves which form a complete orthogonal system of eigenfunctions in the absolutely-continuous subspace of $\mathbf{L}$ In particular the scattered wave

$$\Psi := \left(\Psi^1(x),\ \psi^1(x_1), \psi^1(x_2),\ ...\psi^1(x_N)\right),$$

iniciated by the incoming plane wave e^{-ikx_1} in the first channel (on the wire attached to a_1) has the form:

$$\psi_s^1(x_s) = \delta_{1,s}e^{-ikx_s} + S_{s,1}e^{ikx_s},\ x_s \in \Gamma_s,$$

$$\Psi^1(x) = 2\beta^{-1} < \vec{\bar{G}}_\lambda(x), \left[\frac{1}{ik\beta^2} - Q\right]^{-1} \vec{\delta}_1,\ x \ \in \Omega,$$

where $S_{s,t}$ is the Scattering Matrix calculated by the formula

$$S = \frac{\frac{I}{ik\beta^2} + Q}{-\frac{I}{ik\beta^2} + Q} \tag{25}$$

Proof of this statement exactly follows the pattern of [2]. In particular the explicite expression for the scattered waves $\{\Psi_1, \psi_{1,1}, \psi_{1,2}, \dots \psi_{1,N}\}$ iniciated by plane wave in the first channel Γ_1 and the formulae for the elements $S_{s,1}$ of the Scattering marix is derived from the anzatz

$$\psi_s^1(x_s) = \delta_{1,s}e^{-ikx_s} + S_{s,1}e^{ikx_s},\ x_s \in \Gamma_s,$$

$$\Psi^1(x) = \sum_s A_{1,s}G_\lambda(x, a_s),$$

when inserting them into the boundary conditions and using the connection between the regularized boundary values and singular amplitudes defined by Q-matrix, see(16).

3 Manipulation of electron current in resonance case

.

The expression for effective conductance ${\rho_s}^{-1}$ of an elementary scatterer characterized by the transmission coefficient T was suggested by R. Landauer [6] in form ${\rho_s}^{-1} = (e^2/h)|T|^2/(1-|T|^2)$ which gives the quantum-mechanical conductance $\rho^{-1} = (e^2/h)|T|^2$ if combined with the basic conductance of the quantum wire ${\rho_0}^{-1} = (e^2/h)$ in accordance with the Matiessen rule $\rho = \rho_0 + \rho_s$. This means, that for all but two quantum wires blocked we may obtain the conductance of the quantum domain from Landauer formula, if the corresponding transmission coefficient is calculated. Thus the problem of conductance is reduced to the calculation of the scattering matrix.

We shall do all cpectral calculations for the dimensionless equation in the unit disc, and then choose physical parameters using proper change of variables, see below . the end of this section.

In [2] the scattering matrix is calculated in resonance case when the Fermi-level E_g in the wires Γ_s coincides with a simple *resonance* eigenvalue λ_0 of the nonperturbed operator L on the domain. Assuming that the interaction between the wires and the domain in weak, $\beta >> 1$, we calculate approximately the transmission coefficients $S_{s,1}$ from the wire Γ_1 to the wire Γ_s in terms of values of the resonance eigenfunction at the points of contact. Let us denote by $\vec{\varphi}_0$ a vector in the auxillary channel space E combined of the values of the normalized resonance eigenfunction at the points of contact

$$\vec{\varphi}_0 = (\varphi_0(a_1),\ \varphi_0(a_2),\ \dots \varphi_0(a_N))$$

and by P_0 the orthogonal projection in E onto $\vec{\varphi}_0$:

$$P_0 h = \frac{< \vec{\varphi}_0, h >_E}{|\vec{\varphi}_0|^2}, P_0^{\perp} = I_E - P_0.$$

Due to the basic Lemma 1 , see (17)the separation of singularity in Q-matrix at λ_0 and in the denominator of the scattering matrix is possible:

$$[Q(\lambda) - \frac{1}{ik\beta^2}] =$$

$$\frac{|\vec{\varphi}_0|^2}{\lambda_0 - \lambda} P_0 - \frac{1}{ik\beta^2} + P_0 K_0 P_0 + P_0 K_0 P_0^{\perp} +$$

$$P_0^{\perp} K_0 P_0 + P_0^{\perp} K_0 P_0^{\perp}. \tag{26}$$

This gives the following asymptotics for Scattering Matrix in resonance case for weakening boundary conditions:

Theorem 3.1 *The scattering matrix S^{β} of the operator $\mathbf{L}_{\beta}$ for the weakening boundary condition $\beta \to 0$ has in generic case the following asymptotics at the simple resonance eigenvalue:*

$$S(k) = -I - 2ik\beta^2 K_0 + (I + ik\beta^2 K_0) \frac{2k\beta^2 |\vec{\varphi}_0|^2}{k\beta^2 |\vec{\varphi}_0|^2 + i(\lambda_0 - \lambda)} P_0 + O(|\beta|^4) \approx \tag{27}$$

$$-I + \frac{2k\beta^2 |\vec{\varphi}_0|^2}{k\beta^2 |\vec{\varphi}_0|^2 + i(\lambda_0 - \lambda)} P_0 + o(|\beta|^2)$$

Proof This result may be derived from the previous expression for the Scatterin Matrix (25) in channel space with use of the decomposition (17) of Q-matrix. It also follows the pattern of [2].

□

It follows from the formula (27) that the transmission coefficient $S_{1s}(k)$ from the wire Γ_1 to the wire Γ_s for resonance energy $k^2 = \lambda_0$ is approximately equal to

$$2 \frac{\bar{\varphi}_0(a_s) \varphi_0(a_1)}{\sum_r |\varphi_0(a_r)|^2}, \tag{28}$$

hence it vanishes for all s such that $\varphi_0(a_s) = 0$.

The main objective of actual paper is to choose the contact points $\{a_s\}$ on the unit circle and the intensity of the homogeneous field ε such that the switching of electron current from one direction to another may be manipulated by the direction of the vector e only. It is clear, that for constant electric field oriented along the vector e all eigenfunctions of the nonperturbed operator may be represented as functions of the polar coordinates r, θ, where θ is the asimuth with respect to the vector e, so each eigenfunction is rotated by the angle $\delta\theta$ together with the vector e. This observation shows that the problem of switching the electron's current will be solved if we may find the intensity ε such that some zeroes b_s of the resonance eigenfunction on the boundary of the unit disc Ω satisfy the

condition $\frac{|b_s-b_t|}{|b_s-b_r|}=2$. Then attaching the wires to the unit circle at the points a_2, a_3, a_4 such that $|a_2-a_3|=|a_3-a_4|=|b_s-b_r|$ we may choose the direction of the vector e such that some zeroes of the corresponding resonance eigenfunction coincide either with a_2, a_3 or with $a,3$, a_4. or with a_2, a_4 and at the same time $\varphi_0(a_1)$, $\varphi_0(a_4)\neq 0$ in the first case and $\varphi_0(a_1)$, $\varphi_0(a_2)\neq 0$ i the second case, and $\varphi_0(a_1)$, $\varphi_0(a_3)\neq 0$ in the third case. Then the only essential transmission coefficient for resonance energy will be S_{14} in the first case, or S_{13} in the second case, or S_{13} in the last case.

Using Mathematica we succeded choosing the intensity $\varepsilon=3.68$ such that the eigenfunction which corresponds to the second smallest eigenvalue 3.41 of the corresponding Schrödinger operator in the unit disc with Neumann boundary conditions has only two zeroes on the unit circle wich divide the circle in ratio $2\div 1$. Then attaching the wires at the points with asimuth 0, $\pm\frac{\pi}{3},\pi$ we obtain the pattern of contact points which satisfies required properties, see fig. $1,2,3$ so that we may administer the flow of electrones from the ray Γ_1 to only one of the rays Γ_2, Γ_3 or Γ_4. banning two complementary rays by adjusting the direction of the field V in such a way that both zeroes of the resonance eigenfunction φ of the operator L will coincide with a_2 *and* a_3 or a_2 *and* a_4 or a_3 *and* a_4 - so that only one ray (Γ_4 or Γ_3 or Γ_2 respectively) will be allowed for the flow of electron (see figure 3.1, 3.2, 3.3 respectively and appendix $for_print_ex.nb$) The control over the flow is carried out by the direction e of electrostatic field $V=\varepsilon<x,e>$ which can be changed ad arbitrium. We assume below that this direction defines the reference point for θ so that $\theta=0$ correspondes to the point of the lowest potential (see fig.2). The formula (28) shows that we really may manipulate in this way the quantum current across the domain choose the vector e such that the transition coefficients

$$S_{1k}\approx 0\begin{cases}\text{for } k=2,3\ ;\ \text{and } S_{14}\neq 0\\ \text{or for } k=2,4\ ;\ \text{and } S_{13}\neq 0\\ \text{or for } k=3,4\ ;\ \text{and } S_{12}\neq 0\end{cases}$$

Now we discuss the change of variables which may reduce the real problem to the problem for dimensionless equation. In reality we should consider dynamical processes described by the two-dimentional Schrödinger equation written in polar coordinates with real potential $V=\varepsilon rcos(\theta)+V_0$:

$$(-\frac{\hbar^2}{2m_e}\Delta\Psi+(\mathcal{E}rcos(\theta))+V_0)\Psi=E_g\Psi \tag{29}$$

with the Neumann boundary condition

$$\frac{\partial\Psi}{\partial n}|_R=0$$

in a circular domain radius R on the surface of the narrow-gap semiconductor with effective electron-mass m_e, Fermi level E_g and the potential shift V_0. The radius R should be choosen such that $2R$ are less or equal to the free path of the electron, and V_0 should be choosen such that E_g is exactely equal to the resonanse energy. The typical values of these parameters are given in the table (**??**) in section 1.

In fact we may reduce the spectral analysis of the real equation (29) to the spectral analysis of the corresponding dimensionless equation on the disc radius $r=1$

$$-\Delta\Psi+\varepsilon rcos(\theta)\Psi=\lambda\Psi \tag{30}$$

with Neumann boundary condition at the boundary:

$$\frac{\partial \Psi}{\partial n}|_{r=1} = 0$$

and obtain the recommended values of the parametars from the corresponding change of variables.

Really, by the first step we transform the real equation just by division through $\frac{\hbar^2}{2m_e}$,followed by the change of variable $r \to \xi = \frac{r}{R}$, and then one more division by R_{-2}. This results in dimensionless equation for properly redefined eigenfunction $\varphi_0(\xi, \theta) = \Psi(x, \theta)$

$$-\Delta_\xi \varphi_0 + \mathcal{E}\frac{2m_e R^3}{\hbar^2}|\xi|\cos\theta\varphi_0 = (E_g - V_0)\frac{2m_e R^2}{\hbar^2}\varphi_0 \tag{31}$$

in the unit disc with the Neumann boundary condition at the boundary.

4 Perturbation procedure

We develop the perturbation prosedure for the dimensionsless operator

$$L\varphi = -\Delta_\xi \varphi + \varepsilon\xi\varphi$$

in the unit disc with Neumann boundary condition using the representation of it in the form of indefinite matrix in $\mathbf{l}_2$ with respect to the basis of normalized eigenvectors Φ_{ns} of the *non-perturbed operator*

$$-\Delta_\xi \Phi^{c,s}_{ns} = (k^s_n)^2 \Phi^{c,s}_{ns},$$

which may be constructed in explicite form :

$$\Phi^c_{ns} = \frac{J_n(k^s_n r)cos(n\phi)}{(\int_0^1 |J_n(k^s_n r)|^2 r dr^+ \pi)^{1/2}},\ n = 1.2, \dots$$

$$\Phi^c_{0s} = \frac{J_0(k^s_0 r)}{(\int_0^1 |J_n(k^s_n r)|^2 r dr^+ 2\pi)^{1/2}},\ n = 0,$$

$$\Phi^s_{ns} = \frac{J_n(k^s_n r)sin(n\phi)}{(\int_0^1 |J_n(k^s_n r)|^2 r dr^+ \pi)^{1/2}},\ n = 1.2, \dots$$

Here J_n is n-th Bessel function , and k^s_n is s-th root of the first derivative J'_n of J_n. When using this basis the perturbed operator looks as an orthogonal sum of two block-symmetric matrices $\mathcal{A}^c \oplus \mathcal{A}^s$, the first addenda coresponding to the cosine-part of the basis (including $n = 0$), the second one corresponding to the sine-part of the basis ($n > 0$). The second addend $\mathcal{A}^s$ coincides in fact with the submatrix of the first addend for $n \geq 1$. For this reason we calculate now the first addend $\mathcal{A}^c$ only. It may be represented as a sum of the diagonal matrix $\mathcal{A}^{diag} = \mathrm{diag}(k^s_n)^2$ which corresponds to the nonperturbed operator and the perturbation V caused by the homogeneous field:

$$\mathcal{A} = \mathcal{A}^{diag} + V$$

$$\begin{pmatrix} A_{00}+V_{00} & V_{01} & 0 & 0 & ... \\ V_{10} & A_{11}+V_{11} & V_{12} & 0 & ... \\ 0 & V_{21} & A_{22}+V_{22} & V_{23} & ... \\ . & . & . & . & ... \end{pmatrix}.$$

Here $V_{ik} = V_{ki}^{+}$ and A_{ii} are infinite diagonal blocks with elements

$$A_{ii}^{jj} = (k_i^j)^2$$

$$V_{01}^{st} = \frac{\varepsilon}{\sqrt{(2)}} \frac{\int_0^1 J_1(k_1^s r) J_0(k_0^t r) r^2 dr}{\left(\int_0^1 [J_0(k_0^t r)]^2 r dr\right)^{1/2} \left(\int_0^1 [J_1(k_1^t r)]^2 r dr\right)^{1/2}}$$

$$V_{nm}^{st} = \frac{\varepsilon}{2} \frac{\int_0^1 J_n(k_n^s r) J_m(k_m^t r) r^2 dr}{\left(\int_0^1 [J_n(k_n^t r)]^2 r dr\right)^{1/2} \left(\int_0^1 [J_m(k_m^t r)]^2 r dr\right)^{1/2}}, \quad m = n \pm 1$$

We know that all the eigenvalues of the non-perturbed operator have multiplicity 2 except ones which correspond to the constant angular factor, because for any $\lambda = (k_n^s)^2$ there are 2 eigenfunctions:

$$\frac{J_n(k_n^s r)\cos(n\phi)}{(\int_0^1 |J_n(k_n^s r)|^2 r dr^{+}\pi)^{1/2}}$$

and

$$\frac{J_n(k_n^s r)\sin(n\phi)}{(\int_0^1 |J_n(k_n^s r)|^2 r dr^{+}\pi)^{1/2}}$$

Having in mind the future estimates of errors of the perturbation procedure it is convinient to rearrange the matrix A in the following way. We consider the matrix A as a set of infinite rows, each one containing one "diagonal" element $(k_n^s)^2$. One may deduce easily from the properties of Bessel functions that the roots k_n^sdepend monotonically of both indices: $k_n^s < k_n^t$, if $s < t$, and $k_n^s < k_m^s$, if $n < m$. So, for any fixed positive number M we may find a curve $\{n, s\}_M$ which divides the lattice Z_2 such that $k_n^s \leq M$ and for any m, t , $m > n$ and $t > s$ holds: $(k_m^t)^2 > M$ (see for instance fig.4). Now we rearrange all rows and columns in the order of increasing (non decreasing) "diagonal" elements k_n^s. We denote the rearranged matrix by $\mathbf{A}$ and it's "diagonal" submatrix by $\mathbf{A}^{diag} := \mathrm{diag}(k_n^s)^2$ .Now we have $\mathbf{A}_{ll}^{diag} < \mathbf{A}_{l+1\ l+1}^{diag}$. So for any fixed $M_{_N}$ we may find some finite-dimensional subspace $E_{_N}$ and the corresponding block $\mathbf{A}_{_{NN}}$, whose "diagonal elements" are not greater than than $M = M_{_N}$. The block acting in orthogonal complement $E_{_N}^{\perp}$ we denote by $\mathbf{A}_{_{N^\perp N^\perp}}$ so that the rearranged matrix will look like

$$A = \begin{pmatrix} \mathbf{A}_{_{NN}} & 0 & 0 \\ & V_{_{NN^\perp}} & 0 \\ 0 \quad V_{_{N^\perp N}} & & \mathbf{A}_{_{N^\perp N^\perp}} \\ 0 \quad 0 & & \end{pmatrix}$$

with all "diagonal elements" $\mathbf{A}_{_{N^\perp N^\perp}}$ greater then $M_{_N}$.

We may represent $\mathbf{A}_{_{N^\perp N^\perp}}$ as a sum of the diagonal matrix $\mathbf{A}^{diag}_{_{N^\perp N^\perp}}$ and a bounded matrix $V_{_{N^\perp N^\perp}} = P_{_{N^\perp}} V P_{_{N^\perp}}$.

$$\mathbf{A}_{_{N^\perp N^\perp}} = \mathbf{A}^{diag}_{_{N^\perp N^\perp}} + V_{_{N^\perp N^\perp}}$$

where

$$V_{N^\perp N^\perp} = P_{N^\perp} V P_{N^\perp}$$

Our goal is to find Ψ - eigenvectors of $\mathbf{A}$.

$$\mathbf{A}\Psi^s = \lambda^s \Psi^s \tag{32}$$

In fact shall find the eigenvalues μ_N and eigenvectors ψ_N of a finite matrix $\mathbf{A}_{NN}$

$$\mathbf{A}_{NN}\psi^s_N = \mu^s_N \psi^s_N \tag{33}$$

and prove that the difference

$$\Psi^s - \psi^s_N$$

is assymptotically small for easch s (fixed) when $N \to \infty$. Here we assume that the index s numerates the eigenvectors and eigenvalues μ^s_N of the matrices $\mathbf{A}$, $\mathbf{A}_{NN}$ in the monotonically increasing order: $\mu^s_N \leq \mu^{s+1}_N$.

Theorem 4.1 *When arranging all eigenvalues μ^s_N of A_{NN} in an increasing order so that μ^1_N is the smallest one, and do the same to the eigenvalues λ^s of A then the following correspondance rule is true for large values of N. If λ^s is the s-th eigenvalue of $\mathbf{A}$ which is isolated and simple.*

$$\mathbf{A}\Psi^s = \lambda^s \Psi^s,\ dist(\lambda_s, \lambda_t) = \delta_s.$$

Then for any large M there exist a subspace E_N, $N = N(M)$ $dim E_N = N$ and the block $\mathbf{A}_{N\,N}$ has all "diagonal" elements less than M, and all "diagonal" elements of the complementary diagonal block $\mathbf{A}^{diag}_{N\,N}$ are not less than M. Moreover, if μ^s_N is the eigenvalue number s of of the block $\mathbf{A}_{N\,N}$, then for large N it is also isolated and simple and

$$lim_{N\to\infty}\mu^s_N = \lambda^s$$

and the eigenfunction ψ^s_N of the block-matrix $\mathbf{A}_{N\,N}$ tends to the einenfunction of $\mathbf{A}$

$$lim_{N\to\infty}\psi^s_N = \Psi^s$$

Proof For given M consider the the orthogonal decomposition of the whole Hilbert space into orthogonal sum $E_N \oplus E_{N^\perp}$ and the corresponding orthogonal projections P_N, $P_{N^\perp}$, $P_N \oplus P_{N^\perp} = I$. The operator $\mathbf{A} = \mathbf{A}^{diag} + V$ may be represented in block-form as

$$\mathbf{A} = P_N \mathbf{A} P_N + P_N V P_{N^\perp} + P_{N^\perp} V P_N + P_{N^\perp} \mathbf{A}^{diag} P_{N^\perp} + P_{N^\perp} V P_{N^\perp}. \tag{34}$$

Here $P_N \mathbf{A} P_N = \mathbf{A}_{N\,N}$, $P_{N^\perp} \mathbf{A}^{diag} P_{N^\perp} = \mathbf{A}^{diag}_{N^\perp N^\perp}$, and

$$P_{N^\perp} V P_N = V_{N^\perp N} = \left(P_{N^\perp} V P_N\right)^+ = \left(V_{N\,N^\perp}\right)^+,$$

Let us fix an eigenvalue λ^s of $\mathbf{A}$ and choose $M >> \lambda^s$. We may decompose the eigenfunction of $\mathcal{A}$ into the sum of two components

$$\Psi^s = \Psi^s_N + \Psi^s_{N^\perp}$$

in E_{N} and $E_{N}^{\perp}$ respectively. Now the equation (32) can be written as

$$\left\{ \begin{array}{l} \mathbf{A}_{NN}\Psi_{N}^{s} + V_{NN^{\perp}}\Psi_{N^{\perp}}^{s} = \lambda^{s}\Psi_{N}^{s} \\ V_{N^{\perp}N}\Psi_{N}^{s} + \mathbf{A}_{N^{\perp}N^{\perp}}^{diag}\Psi_{N^{\perp}}^{s} + V_{N^{\perp}N^{\perp}}\Psi_{N^{\perp}}^{s} = \lambda^{s}\Psi_{N^{\perp}}^{s} \end{array} \right. \tag{35}$$

It is clear that $(\mathbf{A}_{N^{\perp}N^{\perp}}^{diag} - \lambda I_{N^{\perp}})^{-1}$ is a small operator if $|\lambda| << M$,

$$||(\mathbf{A}_{N^{\perp}N^{\perp}}^{diag} - \lambda I_{N^{\perp}})^{-1}|| \leq \frac{1}{M - |\lambda|}.$$

So $\Psi_{N^{\perp}}^{s}$ can be represented as follows:

$$\Psi_{N^{\perp}} = -(\mathbf{A}_{N^{\perp}N^{\perp}}^{diag} - \lambda I_{N^{\perp}} + V_{N^{\perp}N^{\perp}})^{-1}V_{N^{\perp}N}\Psi_{N}^{s},$$

where

$$||(\mathbf{A}_{N^{\perp}N^{\perp}}^{diag} - \lambda I_{N^{\perp}} + V_{N^{\perp}N^{\perp}})^{-1}|| \leq \frac{1}{M - |\lambda| - |\varepsilon|},$$

since $|V| = |\varepsilon|$. Hence Ψ_{N}^{s} satisfies the equation:

$$(\mathbf{A}_{NN} - \lambda^{s}I)\Psi_{N}^{s} - V_{NN^{\perp}} \times (\mathbf{A}_{N^{\perp}N^{\perp}}^{diag} - \lambda^{s}I_{N^{\perp}} + V_{N^{\perp}N^{\perp}})^{-1}V_{N^{\perp}N}\Psi_{N}^{s} = 0.$$

The operator $V_{NN^{\perp}} \times (A_{N^{\perp}N^{\perp}} - \lambda I_{N^{\perp}} + V_{N^{\perp}N^{\perp}})^{-1} \times V_{N^{\perp}N}$ is small :

$$||V_{NN^{\perp}}(\mathbf{A}_{N^{\perp}N^{\perp}} - \lambda I_{N^{\perp}} + V_{N^{\perp}N^{\perp}})^{-1}V_{N^{\perp}N}|| \leq \frac{|\varepsilon|^{2}}{M - \lambda - |\varepsilon|}.$$

Further we shall use the notation:

$$V_{NN^{\perp}} \times (\mathbf{A}_{N^{\perp}N^{\perp}} - \lambda I_{N^{\perp}} + V_{N^{\perp}N^{\perp}})^{-1} \times V_{N^{\perp}N} := R_{N}(\lambda)$$

Then the equation for Ψ_{N}^{s} in E_{N} may be represented as

$$\left[\left(\mathbf{A}_{NN} - \lambda^{s}I\right) - R_{N}(\lambda^{s})\right]\Psi_{N}^{s} = 0 \tag{36}$$

The operator $\left[\left(\mathbf{A}_{NN} - \lambda I\right) - R_{N}(\lambda)\right] := [\mathbf{A}]_{\mathbf{N}}(\lambda)$ may be estimated when λ lies on a circle C_{s} radius $\frac{\delta_{s}}{4}$ centered at λ_{s}.

Really, the explicite expression for the resolvent $\Psi = [\mathbf{A} - \lambda I]^{-1}f$ of the operator $\mathbf{A}$ may be obtained as a solution of the the nonhomogeneous equation

$$[\mathbf{A} - \lambda I]\Psi = f,$$

or in decomposed form $\Psi = \Psi_{N}^{s} + \Psi_{N^{\perp}}^{s}$, $f = f_{N} + f_{N^{\perp}}$ with respect to the splitting of the space: $E_{N} \oplus E_{N^{\perp}}$:

$$\left\{ \begin{array}{l} \mathbf{A}_{NN}\Psi_{N}^{s} + V_{NN^{\perp}}\Psi_{N^{\perp}}^{s} - \lambda\Psi_{N}^{s} = f_{N} \\ V_{N^{\perp}N}\Psi_{N}^{s} + \mathbf{A}_{N^{\perp}N^{\perp}}^{diag}\Psi_{N^{\perp}}^{s} + V_{N^{\perp}N^{\perp}}\Psi_{N^{\perp}}^{s} - \lambda\Psi_{N^{\perp}}^{s} = f_{N^{\perp}}. \end{array} \right. \tag{37}$$

Solving this equation as in ([9]) we obtain in particular:

$$(\mathbf{A}_{NN} - \lambda^s I)\Psi^s_N - V_{NN^\perp} \times (\mathbf{A}^{diag}_{N^\perp N^\perp} - \lambda^s I_{N^\perp} + V_{N^\perp N^\perp})^{-1} V_{N^\perp N} \Psi^s_N +$$

$$V_{NN^\perp} (\mathbf{A}^{diag}_{N^\perp N^\perp} - \lambda^s I_{N^\perp} + V_{N^\perp N^\perp})^{-1} f_{N^\perp} = f_N, \tag{38}$$

which means that the operator $[\mathbf{A}]^{-\mathbf{1}}_{\mathbf{N}}(\lambda)$ is exactely the block of the resolvent of $[\mathbf{A} - \lambda I]^{-1}$ in E_N:

$$P_N [\mathbf{A} - \lambda I]^{-1} P_N = [\mathbf{A}]^{-\mathbf{1}}_{\mathbf{N}}(\lambda).$$

Then from general fact concerning selfadjoint operators we obtain the estimate of the inverse via the distance of λ from the spectrum $\sigma(\mathbf{A})$ of operator A:

$$||[\mathbf{A}]^{-\mathbf{1}}_{\mathbf{N}}(\lambda)|| \leq \frac{\mathbf{1}}{\mathbf{dist}(\lambda,\ \sigma(\mathbf{A}))}. \tag{39}$$

In particular this estimate is true for λ lying on the circle $C_s = C_{\lambda_s, \frac{\delta_s}{4}} = \{|\lambda - \lambda_s| = \frac{\delta_s}{4}\}$, so that

$$||[\mathbf{A}]^{-\mathbf{1}}_{\mathbf{N}}\ \mathbf{R}_{\mathbf{N}}(\lambda^{\mathbf{s}})|| \leq \frac{\mathbf{4}|\varepsilon|^{\mathbf{2}}}{\delta_{\mathbf{s}}(\mathbf{M} - |\varepsilon| - |\lambda|)} \to \mathbf{0} \tag{40}$$

for s fixed, $\lambda \in C_{\lambda_s, \frac{\delta_s}{4}}, M \to \infty$.

Consider now the spectral problem in E_N for the operator $\mathbf{A}_{NN}$ *as a perturbation* of the spectral problem (36) for $\mathbf{A}$, assuming that $||R_N(\lambda)|| << 1$. We may choose an eigenvalue μ_N of A_{NN} which is the closest to λ^s and prove that it is simple and isolated for M large enough.

$$(\mathbf{A}_{NN} - \mu^t_N I)\psi^t_N = 0 \tag{41}$$

Comparing the operator-function $[\mathbf{A}_N](\lambda) = \left[\left(\mathbf{A}_{NN} - \lambda I\right) - R_N(\lambda)\right]$ staying in the reduced to E_N spectral problem (36) for the operator $\mathbf{A}$ and the vector-function $\left(\mathbf{A}_{NN} - \lambda I\right)$ staying in the spectral problem (**??**) for the operator $\mathbf{A}_{NN}$ we see that the ratio of them

$$I - \frac{I}{[\mathbf{A}_N](\lambda)} R_N(\lambda)$$

is an invertible operator for large M since the second term in the last formula was estimated on a circle C_s as (40) Then from the operator version of the Rouchet theorem ([18]) we see that for M large enough both spectral problems have the same total multiplicity of eigenvalues in the circle C_s. Hence the spectral problem (**??**) for large M has exactely *one* eigenvalue inside C_s so that μ_N is unique and simple.

The same statement remains true for neighbouring eigenvalues of $\mathbf{A}$, and hence the corresponding neighboring eigenvalues $\lambda_{s-1},\ \lambda_{s+1}$ of the operator $\mathbf{A}_{NN}$ sit in some small δ-neighborhoods of them $\delta < \frac{\delta_{s\pm1}}{4}$, for large M , though they may be *not* simple, if $\lambda_{s-1},\ \lambda_{s+1}$ are not simple. Still the distance of them to μ_N is not less than $frac\delta_s 2$, since we may assume $\delta < \delta_s$.

Now we estimate the error we make using the eigenvalues and eigenfunctions of the operetor $\mathbf{A}_{NN}$ instead the eigenvalues and eigenfunctions of the operator $\mathbf{A}$. Note first

that directly from the equation (35) follows, that the complementary component $\Psi^s_{N^\perp}$ of the eigenfunction is small for large M. Hence to derive the announced result we should proof that $\Psi^s_N - \psi_N$ is small.

Let us represent Ψ^s_N as a sum of the eigenfunction ψ_N , which corresponds to the eigenvalue μ_N and some (eventually - small) vector $\delta\psi$

$$\Psi^s_N = \psi_N + \delta\psi$$

which is orthogonal to ψ_N. We may decompose the operator $\mathbf{A}_{NN}$ as an orthogonal sum

$$\mathbf{A}_{NN} = \mu_N P_{\mu_N} + \hat{\mathbf{A}}_{NN} \tag{42}$$

where

$$\hat{\mathbf{A}}_{NN} = \sum_{\mu^t_N \neq \mu_N} \mu^t_N P_t$$

is the component of the operator $\mathbf{A}_{NN}$ in the orthogonal complement of ψ_N. Then due to the separation of the eigenvalues of $\hat{\mathbf{A}}_{NN}$ proven before we have

$$||(\hat{\mathbf{A}}_{NN} - \mu_{NN})^{-1}|| << max_{\mu_N \neq \mu_N} \frac{1}{|\mu_N - \mu^t_N|} \leq \frac{2}{\delta_s} \tag{43}$$

Using this representation of Ψ^s_N we can rewrite (36) in the following way:

$$(\mathbf{A}_{NN} - \lambda^s I)(\psi_N + \delta\psi) - R(\psi_N + \delta\psi) = 0$$

Considering (42) this leads to

$$(\mu_N - \lambda^s)\psi_N + (\hat{\mathbf{A}}_{NN} - \lambda^s)\delta\psi - R\psi_N - R\delta\psi = 0. \tag{44}$$

Now we will look after $(\mu^s_N - \lambda^s) := \delta\lambda$ and $\delta\psi$. On applying P_s and $P^\perp_s$ to (44) we obtain consequently:

$$\delta\lambda = \langle P_s R(\lambda^s)\psi_N, \psi_N \rangle + \langle R\delta\psi, \psi_N \rangle \tag{45}$$

$$\delta\psi = [\hat{\mathbf{A}}_{NN} - \lambda^s I - P^\perp_s R(\lambda^s) P^\perp_s]^{-1} P^\perp_s R(\lambda^s)\psi_N. \tag{46}$$

Here $[\hat{\mathbf{A}}_{NN} - \lambda^s I - P^\perp_s R(\lambda^s) P^\perp_s]$ is also invertible if $R(\lambda^s)$ is small, because the operator $[\hat{\mathbf{A}}_{NN} - \lambda^s I]^{-1}$ may be estimated by $2\max_{s\neq t}\frac{1}{|\lambda^s - \lambda_t|} = \frac{2}{\delta_s}$, also due to the separation results proven above, (see (**??**),)43)). By substituting (46) to (45) we obtain for large M

$$\delta\lambda \approx \langle P_s R(\lambda^s)\psi_N, \psi_N \rangle$$

and similar statement for $\delta\psi$:

$$\delta\psi \approx [\hat{\mathbf{A}}_{NN} - \lambda^s I]^{-1} P^\perp_s R(\lambda^s)\psi_N$$

□

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