RESONANCE QUANTUM SWITCH: SEARCH FOR WORKING PARAMETERS

N.T. Bagraev, A.B. Mikhailova, B.S. Pavlov, L.V. Prokhorov, A.M. Yafyasov

1 A.F. Ioffe Physico-Technical Institute, St. Petersburg, 194021, Russia.
2 V.A. Fock Institute of Physics, St. Petersburg State University, St. Petersburg, 198504, Russia
3 Department of Mathematics, University of Auckland, Private Bag 92019, Auckland, New Zealand.

Abstract
Design of a three-terminal Quantum Switch is suggested in form of a network consisting of a circular quantum well and four semi-infinite single mode quantum wires attached to it. It is shown that in resonance case, when the Fermi level in the wires is close to some energy level in the well, the magnitude of the governing electric field on the well may be specified in such a way that the quantum current across the switch from the up-leading wire to the outgoing wires (terminals) can be controlled via rotation of the orthogonal projection of the governing electric field onto the plane of the device. The details of design of the switch are chosen in dependence of desired working temperature, available Fermi level and effective mass of electron. The speed of switching is estimated. A solvable model of the switch in form of a one-dimensional graph with a resonance vertex is suggested.

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1 Introduction
Basic problems of quantum conductance were related to Scattering Processes long ago, see [28, 11, 38] and the role of scattering in mathematical design of quantum electronic devices was clearly understood by the beginning of nineties, see [1, 12]. Still the practical design of devices, beginning from the classical Esaki diode [54] up to modern types, see for instance [14], was based on the resonance of energy levels rather than on resonance properties of the corresponding wave functions. Importance of the interference in mathematical design of devices was noticed in [17, 2] and intensely studied in [38, 18, 24, 22], see also recent papers [48, 55].

Modern experimental technique already permits to observe resonance effects caused by details of the shape of the resonance wave functions, see [6, 7, 8, 53]. We propose using of these effects as a natural tool for manipulation of the electron’s current in the quantum switch with one input wire and three terminals.

Our problem on mathematical design of a three-terminal Quantum Switch RQS-3 (for triadic logic) appeared first as a Work-Package in the ES-Project (joint with Solvay Institute) "New technologies for narrow-gap semiconductors" ESPRIT-28890 NTCONS, 1998 - 1999. Results of the project were initially formulated in rather mathematical language in [10], for the switch based on the quantum ring, in [32], and later in [33] for the switch based on the quantum well and patented in [39]. Prospects of practical implementation of the devices were discussed in [40]. Note, that an attempt of computation of the quantum current through the Y-junction was also done in recent paper [16], but an important connection between the geometric characteristics of the junction, encoded in the corresponding Dirichlet-to-Neumann map, was not noticed there.

Our initial mathematical idea of the resonance manipulation of the single-mode quantum current was based on an observation from [19]:

The resonance transmission across the quantum system caused by attachment of incoming and outgoing channels is proportional to the products of proper local characteristics of the corresponding resonance eigenfunction of the system at the places where the channels are attached.
Some mathematical aspects of this observation were discussed in papers [32, 33, 42, 34]. In actual paper we describe a parameter regime where the quantum switch works. The Resonance Quantum Switch is formed as a Quantum network Ω on the surface $R^2$ of a semiconductor and consists of a deep quantum well $\Omega_0$ and few equivalent quantum wires $\Omega_1, \Omega_2, \Omega_3, \Omega_4$ attached to it.

The role of Hamiltonian of the corresponding quantum system is played by the one-electron Schrödinger operator $l$, see below in section 2. The potential is constant $V_\infty$ in the wires, linear (corresponding to the macroscopic electric field) on the well and zero on the complement $R^2 \setminus \Omega := \Omega'$ of the network. If the depth of the Fermi level in the wires with respect to the potential on the complement of the network is large enough, see estimates below in sub-section 2.1, one can replace the matching boundary conditions on the border of the network with the complementary domain $\Omega'$ by the homogeneous Dirichlet conditions, at least for electrons with energy close to the Fermi level. We do not assume actually that the wires are thin (see the discussion below in the subsection (2.3) or connection of the wires to the quantum well is weak, but we assume that the dynamics of electrons in the wires is single-mode and ballistic on large intervals of the wires, compared with the size of the geometric details of the construction (the width of the wire or the size of the contacts). We consider the electron's transmission across the well from one wire to another as a Scattering process. It appears that the transmission coefficients can be manipulated via macroscopical electric field applied to the quantum well, see section 5. We aim at the estimation of the temperature stability of the device and the speed of switching in dependence on geometrical details of the construction and properties of selected materials.

Note that it is impossible to construct a solution to the Schrödinger equation on the Quantum network in analytic form. On the other hand the direct computing is non efficient for optimization of the construction because of large number of essential parameters and the resonance switching effect observed only on the triple (or multiple) point in the space of essential physical and geometrical parameters.

Analysis of the one-dimensional Schrödinger equation on the corresponding one-dimensional graph is a comparatively simple alternative of explicit formulae for the solution of the above Scattering problem, but estimation of errors appearing from the substitution of the Quantum network- the “fattened graph”- by the

![Figure 1: Resonance Quantum Switch. The circular quantum well $\Omega_0$ with wires $\Omega_j$, $j = 1, 2, 3, 4$ attached. The modified well $\tilde{\Omega}_0$ has small circular arcs of the circular boundary replaced by the flat bottom sections $\gamma_j$ of the wires.](image)
corresponding one-dimensional graph may be difficult. In mathematical papers [27, 17] the authors study the spectrum of the Schrödinger operator on a compact “fattened graph”. Based on variational approach developed in [10] they noticed that the (discrete) spectrum of Laplacian on a system of finite length shrinking wave-guides width δ attached to the shrinking vertex domain diameter $R = R_\delta$, $\delta^\alpha$, $0 < \alpha < 1$, tends to the spectrum of Laplacian on the corresponding one-dimensional graphs, but with different boundary conditions at vertices, depending on the speed of shrinking.

In distinction from the papers [27, 17] quoted above, our approach to the Schrödinger equation on the “fattened graph”, see [33, 42], is based on analysis of the resonance transmission through the quantum well radius $R$ with few quantum wires width δ attached to it. Assuming that Fermi level is situated on the first spectral band in the wires, we impose additional “chopping off” boundary conditions on the bottom sections of the semi-infinite wires. These condition split the original operator into orthogonal sum of the trivial part $\{\sum_{s=1}^d I_s\}$ in the open channels and a non-trivial part $I_0$ which plays the role of an “Intermediate operator”: $l \to \{\sum_{s=1}^d I_s\} \oplus I_0$. The spectrum of the intermediate operator consists of an absolutely continuous part of varying multiplicity which begins from the second threshold in the wires and a sequence of eigenvalues $\lambda_s^r$ which can accumulate at infinity. The eigenvalues which are sitting on the first spectral band generically give rise to resonances of the Scattering problem on the network and hence define the resonance conductance.

Our main tool is the following approximate formula for the Scattering matrix in terms of eigenfunctions $\varphi_i$ of continuous and discrete spectrum of the Intermediate operator and corresponding eigenvalues:

$$S(\lambda) \approx \frac{i p(\lambda)}{i p(\lambda) - DN_{\lambda}^r} := S_\gamma(\lambda),$$

(1)

where $i p(\lambda)$ is, in simplest case, an exponent from the bounded modes $e^{\pm i p(\lambda)x}$ in open channels, spanned by the corresponding cross-section eigenfunction $e_s$, and

$$DN_{\lambda}^r(\lambda) = \sum_i P_+ \frac{\partial \varphi_i^r}{\partial x_n} \langle P_+ \frac{\partial \varphi_i^r}{\partial x_n} \rangle + \int P_+ \frac{\partial \varphi_i^r}{\partial x_n} \langle P_+ \frac{\partial \varphi_i^r}{\partial x_n} \rangle d\rho(\lambda_i)$$

(2)

is an essential part of the Dirichlet-to-Neumann map of the Intermediate operator $I_0^r$, which contains summation and integration over spectrum $\{\lambda_i\}$ of the Intermediate operator situated on the essential interval of energy $|\frac{\hbar^2}{2m_0} \lambda_i - E_F| < \kappa T$ for given temperature. The operator $P_+$ is a projection $\sum_{s=1}^d e_s \langle e_s \rangle$ onto the subspace $E_+ = \sqrt{\sum_{s=1}^d e_s}$ spanned by the cross-section eigen-functions of open channels on the bottom sections of the wires.

In most interesting case when only one resonance eigenvalue $\lambda_s^r$ is sitting on the essential spectral band, the above formula (1) gives important “one-pole approximation” which is used below for estimation of the working parameters of the switch.

Our paper has the following plan. In the second section we describe the Hamiltonian and supply (in 2.2) some physical motivation supporting the choice of basic parameters and generally motivate our approach. In the third section we formulate the relevant Scattering Problem and announce the formula for the Scattering matrix in terms of the Dirichlet-to-Neumann map (DN-map) of the Intermediate operator. The derivation of this formula is postponed to Appendix, sub-section 10.2. In fourth section we apply the announced formula for estimation of the speed of switching, and derive from it a useful approximate formula which is valid for relatively low temperature - the “one-pole approximation” of the Scattering matrix. In fifth sections we discuss the resonance switching phenomenon. In the section 6 we suggest a procedure of choosing of the working point of the device in dependence on desired working temperature and in the last section 7 we describe a solvable model of the switch in form of a one-dimensional graph with a resonance vertex. In Appendix we supply technical details on DN-map, derive the announced formula for the Scattering matrix and interpret the corresponding one-pole approximation [32] as a Scattering matrix of some solvable model.
2 Design of the switch

Here we provide a preliminary discussion of physical and geometrical limitations of the switch. A basic example is considered in sub-section 2.3.

2.1 Schrödinger equation

Conductance of the network constructed on the surface of the crystallized medium depends on geometry of the network and on the correspondence between the crystal structure and the form and positions of the wires with respect to the geometry of the crystal’s lattice. In simplest case this dependence is encoded in tensor of effective mass of the electron and in basic potentials in the wires and on the well. For instance, on (100)-plane in the Si matrix there are two lower and four upper valleys. For lower valleys effective masses are equal $m_\perp = m_t = 0.190 \, m_0$ across the valley and $m_\parallel = m_e = 0.916 \, m_0$ along the valley, where $m_0$ is the conventional electron mass. On the plane (110) there are four lower valleys with effective masses calculated as $\frac{m_\perp + m_\parallel}{2} = 0.553 \, m_0$, $\frac{2m_\perp m_\parallel}{m_\perp + m_\parallel} = 0.315 m_0$ respectively and two upper valleys with masses $m_t$, $m_e$, $m_t$. For quantum wires formed on the surface of some narrow-gap semiconductors, like CdHgTe, the tensor of effective mass is isotropic, and the value of the effective mass is small, $m_\parallel = m_\perp < < m_0$, see [30] and the table in section 6. In following sections we assume that in case of switch based on Si the effective masses across and along the vares are the same for all wires: $m_\perp = 0.190 \, m_0$ and $m_\parallel = 0.916 \, m_0$ respectively. Note that the resonance switching phenomenon is defined by the geometry of the well, see section 5, and is invariant with respect to the magnitudes of effective masses: the masses may be different in different wires. Though the transmission coefficients depend on effective masses, they can be easily calculated, once the orientation of the wires with respect to the crystal’s structure and the corresponding effective masses are known.

The bottom of the quantum well in a crystallized medium is generally a sophisticated network of valleys. We assume that the fine structure of this pattern permits to replace the corresponding Schrödinger equation with anisotropic effective mass by the standard Schrödinger equation with an average effective mass:

$$-\frac{\hbar^2}{2m} \Delta + V(x) = E \nu u. \quad (3)$$

We assume that quantum dynamics outside the network is generated by similar Schrödinger equation with zero potential on the complement of the network $V_{\text{out}}(x) = 0$, $x \in \Omega'$, $\partial R_2 \setminus \Omega$, and the averaged effective mass for both equations coincides with the conventional electron mass $m_0$. If the Fermi level is deep enough counting from the level of the potential outside the network, compared with the radius of the well:

$$\frac{2m_0(0 - E_f)}{\hbar^2} R^2 = 0.3136 \, (0 - E_f) \, R^2 \gg 1,$$

($R$ measured in angströms and the depth of the Fermi level $(0 - E_f)$ in electron-volts), then for the values of energy $E$ near to the Fermi-level $E_F$, the spectral problem can be reduced to the spectral problem for the corresponding Schrödinger operator on the network $\Omega := \Omega_0 \cup \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_4$ with the mixed boundary condition on the boundary $\partial \Omega$:

$$\frac{\partial u}{\partial n} + \sqrt{\frac{2m(V_{\text{out}} - E_F)}{\hbar^2}} u \bigg|_{\partial \Omega} = 0,$$

or even with zero (Dirichlet homogeneous) boundary condition, if the above ratio is large enough. In this paper we just assume that

$$u \bigg|_{\partial \Omega_0} = 0.$$

The potential $V(x)$ on the quantum well is defined by the macroscopic “governing” electric field $E \nu$ which is constant inside the well, $V(x) = E \nu(x, \nu) + V_0$, where $e$ is the electron charge and the unit vector $\nu$ shows the direction of the field. The magnitude of the field is specified in section 5.

In the wires $\Omega_2$: $-1 < x < \infty$, $0 < y < \delta$ the potential is piece-wise constant

$$V_s(x, y) = \begin{cases} V_\infty + \frac{\hbar^2 \nu^2}{2m_0} & \text{if } -1 < x < 0 \\ V_\infty & \text{if } x > 0, \end{cases}$$

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or constant, $V(x) = V_\infty$, if $l = 0$. The first case corresponds to presence of a split-gate on the initial part $-1 < x < 0$ of the wire, see below, section 3, in second case the split-gate is absent or switched off.

We assume that the tensor of effective mass in the wires is non-trivial: the effective mass across the wire $m^\perp$ and along the wire $m^\parallel$ are different, see the data for Si above, or equal, as for some narrow gap semiconductors. The magnitude of $m^\perp$ defines, up to some shift, the thresholds $\frac{\hbar^2}{2m^\perp} \pi^2 \delta^2$, $l = 1, 2, \ldots$, separating spectral bands in the wires.

We assume that the role of the one-electron Hamiltonian on the network is played by the Schrödinger operator:

$$l = -\frac{\hbar^2}{2m} \Delta + V(x)$$

with potential and tensor of effective mass specified as described above. It is convenient to use the “geometric” form of the corresponding Schrödinger equation with re-normalized spectral parameter $\lambda = p = 2 \frac{m_0}{\hbar^2} [E - V_\infty - \frac{\hbar^2}{2m^\parallel} \pi^2 \delta^2]$. On the well we have:

$$-\frac{1}{m_0} \Delta_x u(x) + \frac{2}{\hbar^2} \left[ V(x) - V_\infty - \frac{\hbar^2}{2m^\parallel} \pi^2 \right] u = \frac{2}{\hbar^2} \left[ E - V_\infty - \frac{\hbar^2}{2m^\parallel} \pi^2 \right] u(x), = \frac{1}{m_0} \lambda u, |x| < R,$$

with a new spectral variable $\lambda$ or $p = \sqrt{\lambda}$, which plays a role of an effective wave-number. The non-dimensional form of the above Schrödinger equation on the well is obtained via change of the space variable $x \to \xi = (\xi_1, \xi_2) = \frac{2}{R} x$:

$$-\frac{1}{m_0} \Delta_\xi u(R\xi) + \frac{2}{\hbar^2} \left[ V(R\xi) - V_\infty - \frac{\hbar^2}{2m^\parallel} \pi^2 \right] u(R\xi) = \frac{2}{\hbar^2} \left[ E - V_\infty - \frac{\hbar^2}{2m^\parallel} \pi^2 \right] u(R\xi) = R^2 \frac{\lambda}{m_0} u(R\xi) := R^2 \frac{\lambda}{m_0} u, |\xi| < 1. \quad (6)$$

The corresponding change of variables on each wire : $x \to \xi = \frac{x}{R}$ along the wire and $y \to \eta = \frac{y}{R}$ across the wire, $0 < y < \delta$, $x > -1$ gives the equation :

$$-\frac{1}{m^\parallel} \frac{d^2 u}{d\xi^2} - \frac{1}{m^\perp} \frac{d^2 u}{d\eta^2} + \frac{2}{\hbar^2} \left[ V - V_\infty - \frac{1}{2m^\parallel} \pi^2 \right] u = \frac{2}{\hbar^2} \left[ E - V_\infty - \frac{\hbar^2}{2m^\perp} \pi^2 \right] u := \frac{R^2}{m_0} \frac{\lambda}{m_0} u, \quad \lambda \equiv \frac{R^2}{m_0} \pi^2. \quad (7)$$

We will use further both geometric and non-dimensional forms of Schrödinger equations in the wires and on the well assuming that each time proper change of variables is also done in the function $u$. We also consider corresponding Schrödinger operators, in particular the Intermediate operator, with specified coefficients and boundary conditions, see the next section 3 and Appendix, section 9.1.

### 2.2 Geometrical and physical limitations

**Spectrum** Our approach to calculation of transmission coefficients is based on introduction of an “Intermediate operator” defined as Schrödinger operator with partial “chopping-off” boundary conditions on the bottom sections of channels, see (21,22) below. These conditions define the Intermediate operator as a Schrödinger operator on the orthogonal complement of the open channels in the wires. If the Fermi level sits on the first spectral band, then the non-trivial part of the intermediate operator on the orthogonal complement of the open channels has a branch of absolutely-continuous spectrum (varying multiplicity)
beginning from the second threshold in the wires, \( \sigma_v^r = \left[ V_\infty + \frac{4\pi e^2}{2m\delta}, \infty \right] \) and, probably, few eigenvalues below the second threshold. Those of them which sit above the first threshold become embedded eigenvalues or are transformed to resonances of the Schrödinger operator on the whole network, when the “chopping-off” boundary conditions \( 21, 22 \) are replaced by the matching boundary conditions in all channels, see \( 23 \) below. Submitting the standard scattering Ansatz to these boundary conditions \( 24 \) we will derive in the next section an explicit expression \( 25 \) for the Scattering matrix in terms of the Dirichlet-to-Neumann map (DN-map, see Appendix, 10.2) of the Intermediate operator. It is shown there that the “partial” DN-map of the Intermediate operator is connected with the standard DN-map of the Schrödinger operator on the quantum well, see the corresponding formula \( 26 \) and the theorem 10.4 in subsection 10.3. In particular the “re-normalized” eigen-values \( \lambda^r \) (of the Intermediate operator ) which are sitting on the first spectral band, between the first and second thresholds, are obtained by minor shifts \( \Delta \) of the eigenvalues \( \lambda_s \) of the Schrödinger operator on the quantum well with zero boundary condition on the whole boundary:

\[
\lambda_s \rightarrow \lambda^r = \lambda_s + \Delta_s.
\]

The deviations of the eigenvalues of the non-dimensional Intermediate operator from the eigenvalues of the corresponding Schrödinger operator on the well with zero boundary conditions are estimated in Appendix, subsection 10.4. For the most interesting case of the circular well the corresponding non-dimensional Schrödinger operator on the well with zero boundary conditions are estimated in Appendix, subsection 9.1:

\[
\lambda_{s} \rightarrow \lambda^r_{s} = \lambda_{s} + \Delta_{s}.
\]

In the remaining part of this section we will not distinguish the spectral data of the Intermediate operator below the second threshold from the spectral data of the Schrödinger operator on the well with zero boundary conditions. We assume temporarily in this section that split gates are absent, \( l = 0 \).

**Leading terms of DN-map** The numerator and denominator of the above approximation \( 11 \) for the Scattering matrix contain the expression for \( 21 \) and the exponent \( i\mathcal{P}I \). If the Fermi level \( E_F \), and hence the energy of electron, sits in the upper part of the first spectral band, then the leading terms in both numerator and denominator of the approximate expression \( 11 \) presented in terms of geometrical variables are: the resonance term

\[
\frac{P_+ \frac{\partial \phi_+}{\partial n}}{\lambda - \lambda_0}
\]

which corresponds to the “resonance energy level”

\[
E_0 = \frac{\hbar^2}{2m} \frac{\pi^2}{\delta^2} + V_\infty + \frac{\hbar^2}{2m_0} \lambda_0 \approx E_F,
\]

closest to the Fermi level \( E_F \), and, probably, the exponent \( i\mathcal{P}(\lambda)I \) which, in simplest case, is proportional to the effective wave-number \( \mathcal{P}(\lambda) = \sqrt{\frac{m_i}{m_0}} p = \sqrt{\frac{m_i}{m_0}} \sqrt{\lambda} \), see Appendix, subsection 9.1:

\[
p_0^2 = \frac{2m}{\hbar^2} \left[ E_0 - V_\infty - \frac{\hbar^2}{2m} \lambda \right].
\]

The subordinate (non- resonance) terms may be estimated by the contribution to \( \mathcal{D}_{calN} \) from the closest to \( E_0 \) “non-resonance” energy level \( E_1 \neq E_0 \):

\[
\frac{P_+ \frac{\partial \phi_+}{\partial n}}{\lambda - \lambda_1},
\]

and by the contribution from the upper branch of the continuous spectrum which begins from the second threshold \( \sqrt{\frac{m_i^2}{\delta^2} \frac{\pi^2}{2m}} + \frac{2m\mathcal{V}}{\hbar} \). This contribution is estimated by the product of the inverse “geometric spacing” at the resonance level \( \rho(\lambda_0) = \min_\gamma |\lambda_0 - \lambda_\gamma| \) and the norm \( ||P_+ \frac{\partial \phi_+}{\partial n}||^2 = C_R \) of the one-dimensional
operator $P_\gamma = P_+ \frac{\partial \gamma}{\partial m}(P_+ \frac{\partial \gamma}{\partial m})$, which stays in the numerator of the fraction (38). It can be estimated as $C_\gamma \leq \tilde{C}R_\gamma^{-\beta}$ with a non-dimensional constant $\tilde{C}$. The constant $\tilde{C}$ is the norm of the corresponding one-dimensional operator for circular quantum well radius $1$, and in the example below it does not exceed 10.

We say, that the width of the wires is relatively small compared with the radius $R$ of the quantum well, if the inverse “re-normalized” spacing on Fermi level is dominated by the non-dimensional effective wave-number $p' = Rp$:

$$\frac{\hbar^2}{2m_0 R^2 p'(E_F)} \ll R \sqrt{\frac{2m_0 |E_F - V_{\infty}| - m^\parallel \pi^2}{\hbar^2}} - m^\parallel \pi^2 - m^\perp \delta^2 := \frac{\gamma_1}{\gamma_2} \frac{m^\parallel}{m_0} p' = \frac{\pi R}{\delta} \sqrt{\gamma_1 \frac{m^\parallel}{m_0}}.$$  \hspace{1cm} (9)

The right side of the above inequality and the “re-normalized” spacing $\frac{2m_0 R^2 p'}{\hbar^2} := p^1$ in the denominator in the left side of the last condition are non-dimensional. The “re-normalized” spacing is actually equal to the spacing on the resonance level $\lambda_0 : \frac{\hbar^2}{2m_0 R^2} R^2 \lambda_0 = E_0 \approx E_F$ of the corresponding non-dimensional Schrödinger equation.

**Temperature** When assuming that the radius $R$ of the quantum well is relatively small, for given temperature, we actually have in mind that the spacing $\rho(E_F) = \min_{s \neq 0} |E_s - E_0|$ of energy levels in the quantum well $\Omega_0$ radius $R$ at the resonance energy level $E_0$ closest to the Fermi level, $E_0 \approx E_F$ (with wires disjoint from the domain) is large compared with temperature:

$$\kappa T < \frac{1}{2} \inf_{E_F, E_s} |E_F - E_s| = \rho(E_0).$$ \hspace{1cm} (10)

Generally, there may be several eigenvalues $E_s = V_\infty \frac{\hbar^2 \pi^2}{2m_0} \lambda_s$ of the Intermediate operator (or the Schrödinger operator on the well) situated on the essential interval of energy centered at the Fermi level $[E_F - \kappa T, E_F + \kappa T]$ divided by the Fermi level $E_F$.

$$E_F - \kappa T \leq E_s \leq E_F + \kappa T.$$ \hspace{1cm} (11)

In this case we neglect the polar terms in the DN-map which correspond to eigenvalues outside the essential interval.

When assuming that the Fermi level $E_F$ is situated in the upper part of the first spectral band $[\frac{\hbar^2 \pi^2}{2m_0 \delta^2} + V_\infty, \frac{\hbar^2 \pi^2}{2m_0 \delta^2} + V_\infty + \frac{4\hbar^2 \pi^2}{2m_0 \delta^2}]$ in the wires, we suppose that $E_F$ divides the first spectral band in ratio $\mu_1 : \mu_2$, $\mu_1 + \mu_2 = 1$, $0 < \mu_2 < \mu_1$

$$E_F = V_\infty + \mu_1 \frac{\hbar^2 \pi^2}{2m_0 \delta^2} + \mu_2 \frac{4\hbar^2 \pi^2}{2m_0 \delta^2}.$$ \hspace{1cm} (12)

Then one can estimate the distances of the Fermi level to the first $\frac{\hbar^2 \pi^2}{2m_0 \delta^2} + V_\infty$ and the second $\frac{4\hbar^2 \pi^2}{2m_0 \delta^2} + V_\infty$ thresholds in the wires respectively as $\mu_1, \mu_2 3 \frac{\hbar^2 \pi^2}{2m_0 \delta^2}$ and the square “effective wave-number” on on Fermi level as $p^2_F = 3\mu_1 \frac{m_0 \pi^2}{m_0 \delta^2}$.

Extending the principle [11] to the continuous spectrum, we will neglect the contribution to DN-map from the continuous spectrum of the Intermediate operator if it does-not overlap with essential spectral interval for given temperature $T$. If the Fermi level sits below the second threshold, this means:

$$\gamma_2 \frac{3 \pi^2 \hbar^2}{2m_0 \delta^2} > \kappa T.$$ \hspace{1cm} (13)

For Si with $m^\perp = 0.19$ and wires width 5 nm this condition estimates the temperature in K as $T < 250K \mu_2$, which means that Nitrogen temperature $77K$ are low enough to neglect in approximate formula for the Scattering matrix the contribution from the second spectral band, if the Fermi level divides the first spectral band in ratio $\mu_1 : \mu_2 = 2 : 1$. For wires width $6mm$ one can neglect the contribution from the continuous spectrum of the Intermediate operator for Nitrogen temperature if the Fermi level is situated in the middle of the first spectral band. Note that the width of the wires as self-assembled patterns on the Si matrix can be already controlled with precision better than 2 nm. [6]
2.3 Example

In anticipation of the discussion of parameter’s regime of the Resonance Quantum Switch in section 6, we consider the most interesting example of the switch, based on a circular quantum well with quantum wires width $\delta = R/2$. Assume that the shift potential $V_0$ in the well is selected such that $V_0 - V_\infty - \frac{\hbar^2}{2m^*} \frac{2\pi^2}{\delta^2} = 0$.

Then the potential of the corresponding non-dimensional Schrödinger equation on the well is just proportional $\langle \xi, \nu \rangle u$. Assume that the re-normalized electric field is selected as $e = 18.86$. Then the eigenfunction of the non-dimensional Schrödinger operator on the quantum well

$$-\Delta_{\xi} u - e(\xi, \nu)u = R^2 p^2 u,$$

which corresponds to the (non-dimensional) resonance eigenvalue $R^2 \lambda_0 = 14.62$ has a special shape which can be used for manipulation of the quantum current, see [33] and the section 5 below.

We assume that $R^2 \lambda_0 = 14.62 = \hat{\lambda}_0$ is the non-dimensional resonance level, $\frac{\hbar^2 \lambda_0}{2m_0} \approx E_F$ in the well with zero boundary conditions. The non-dimensional deviation $\Delta_0 = -0.07$ from the corresponding “shifted” eigenvalue $R^2 \lambda^*_0 = 14.554$ of the intermediate operator is small and is dominated by the non-perturbed spacing - the distance $-2.30$ to the nearest non-resonance eigenvalue 12.32. The above condition [31] remains valid for the Intermediate operator too.

**Small parameter** If the Fermi-level divides the first spectral band in ratio $\gamma_1 : \gamma_2$, then the one-pole approximation is applicable to the switch with “relatively narrow” wires if the condition (14) is fulfilled. In actual case of the switch based on a circular quantum well this condition takes the form:

$$\frac{1}{2.3} \ll \frac{R}{\delta} \pi \sqrt{\frac{m_0^*}{m^*} \mu}, \quad (14)$$

It obviously holds if the width $\delta$ of the wires does not exceed $\frac{R}{2}$, and the Fermi level sits in the middle of the first spectral band $\mu_1 = \mu_2 = 1/2$: It may be reduced in this case to :

$$1 \ll 20 \sqrt{\frac{m_0^*}{m^*} \mu}, \quad (15)$$

which is not restrictive at all in case $\delta < R/2$. Moreover it permits to use the “natural” small parameter $\frac{1}{20} \sqrt{\frac{m_0^*}{m^*} \mu}$ in perturbation procedures in sections 3, 4 and sub-sections 10.2, 10.3.

When formulating the basic condition [31] [34] we deliberately omitted the constant $\hat{C}$ which estimates the norm of the one-dimensional operator in the numerator of the non-resonance polar term of the $D\mathcal{N}_\tau$. In our example the non-dimensional constant $\hat{C}$ is less than 10, see the sub-section 5.2 and [46], hence the accurate estimation of the non-resonance contribution *with regards of the constant $\hat{C} = 10$* still results in “small” parameter (4.4)$^{-1}$:

$$10 \ll 20 \sqrt{\frac{m_0^*}{m^*} \mu} \approx 44. \quad (16)$$

for Si, if $\delta \leq \frac{R}{2}$, which shows the “degree of domination” of the non-resonance contribution by the effective wave-number. For more sophisticated geometry the question on the domination requires accurate calculation.

**Low temperature** Though the condition [31] was initially formulated independently of temperature, we saw that physically this condition is required only for spectrum of the intermediate operator inside the essential interval of energy: $(E_F - \kappa T, E_F + \kappa T)$. In particular, if the condition [33] is fulfilled, this interval does not overlap with upper branches of the absolutely-continuous spectrum:

$$E_F + \kappa T < V_\infty + \frac{\hbar^2}{2m^*} \frac{4\pi^2}{\delta^2}. \quad (17)$$
Then the contribution to the essential part DN-map of the Intermediate operator, and hence to the Scattering matrix, from the upper branches of the absolutely-continuous spectrum can be neglected. If there are no eigenvalues in the essential interval of energy,

$$E_p - \kappa T < E_o < E_p + \kappa T,$$

except the resonance eigenvalue $E_0 = E_p$, that is $|E_p - E_o| \geq \kappa T$ for $t \neq 0$, then only one resonance term remains in the corresponding approximate expression for the DN-map, and hence for Scattering matrix the “one-pole approximation” can be used, see the discussion in section 2. If all these conditions are fulfilled (on the essential interval of energy), then the transmission coefficient from one wire to another exhibits clear resonance properties in single-mode scattering process see the next sections 4, 5. These properties are defined by the shape of the resonance eigenfunction, see the discussion in section 5. In section 4, using the one-pole approximation for the DN-map Scattering matrix, and the presence of the small parameter arising from we calculate the resonances and estimate the speed of switching.

3 Boundary conditions and Intermediate operator.
Scattering matrix.

3.1 Split-gates

We consider a single act of the electron’s transmission from the incoming wire to one of terminals as a scattering process on a quantum network constructed of a circular quantum well $\Omega_0 = \{ x : |x| < R \}$ and several straight quantum wires - the trenches $\Omega_n$ width $\delta$ - attached to it orthogonally centered at the points $a_n$ on the boundary of the well ( $n = 1, 2, 3$ for two-terminal switch RQS-2 and $n = 1, 2, 3, 4$ for three-terminal switch RQS-3). The wire $\Omega_1$ is selected for the input, others are terminals. Positions of the points $a_n$ are chosen to optimize the switching effect, see below, section 5. One may suggest two engineering solutions of the problem of manipulation of the quantum current across the switch. The first may be based on manipulation of the height of barriers $V_{\text{barrier}} = \hbar^2 k^2/2m_0$ on the initial part of the wires $-1 < x < 0$ via the change of the corresponding electric field, thus closing or opening the “split-gates”. This mechanism may be used even in case when the wires are wide enough (not “single mode”). The speed of transition processes in the switch (hence the speed of switching) in this case depends not only on geometry of the network, but is defined by the microscopic properties of the materials and can’t be easily estimated theoretically. Another mechanism is based on the resonance scattering in the switch. It can be applied only to single-mode wires. The speed of switching in second case can be estimated in terms of geometrical parameters of the switch. Though the first mechanism is efficient for manipulating stronger currents, we consider in this paper the second one, based on solution of the resonance scattering problem for the corresponding Schrödinger equation

$$-\hbar^2/2m_0 \Delta u + V(x)u = Eu.$$

3.2 Optimization of design: solvable model versus scanning

If all parameters of the model are chosen, then the above scattering problem can be, at least “in principle”, solved numerically with proper potential $V$ on the whole space when assuming that the potentials and tensor of effective mass on the network. Mathematical theory of the above scattering problem on the network with zero boundary condition is developed in [33, 42, 34]. In actual paper we use presence of the natural small parameter, which permits, practically, to neglect the contribution to the Scattering matrix from the non-resonance eigenvalues. Moreover we may assume that the matching of the solution of the Schrödinger equation on the circular quantum well with the solutions in the rectangular wires may be done on the flat bottom sections just via replacement of the central angle by the corresponding sine due to the condition $\delta/R < 1/2$, $\theta < \pi/6$:

$$\theta - \sin \theta < \frac{\pi}{6} - \frac{1}{2} \approx 0.023,$$
This observation permits to calculate approximately the resonance entrance vectors forming projections in the numerator of polar terms of the DN-map \( \Omega \), see subsection 10.3, and even estimate accurately the error appearing from substitution of the circular quantum well \( \Omega \) by the corresponding “almost circular” modified domain \( \{ \Omega_1 \cup \Omega_2 \cup \ldots \} \) which has flat pieces on the boundary matching the bottom sections of the wires, see [42]. Results of the spectral analysis of the Schrödinger equation on the modified quantum well with flattened pieces at the places of contact with wires, only slightly deviate from ones on the circular one.

Nevertheless neither numerical solution, nor the straightforward experimental search are efficient in course of search of the parameter regime where the Resonance Quantum Switch works, since the space of physical and geometrical parameters of the switch is multi-dimensional. The “working point” of the switch is actually a sort of a “multiple point” which is easy to miss when scanning on one of parameters with other parameters fixed at random. Our search of the working point is based on mentioned above explicit approximate formula (“one-pole approximation”) for the Scattering matrix which permits to obtain preliminary estimation of the working parameters, thus minimizing the task of the random search. The derived approximation is actually an exact Scattering matrix of proper solvable model which is constructed in section 7.

### 3.3 Intermediate operator

In this sub-section we announce an exact formula for the Scattering matrix based on Dirichlet-to-Neumann map of the Intermediate operator. The corresponding elementary calculation is postponed to the subsection 9.2. We derive the formula for the geometric form of the Schrödinger equation on the network, replacing the standard Schrödinger equation (3) on the well \( \Omega \) by

\[
- \frac{1}{m_0} \Delta u + \frac{1}{m_0} V_0(x) u = \frac{1}{m_0} \lambda u, \tag{19}
\]

and on the wires \( \Omega_s \) by

\[
- \frac{1}{m} \Delta u + \frac{1}{m} V_s(x) u = \frac{1}{m} \lambda u, \tag{20}
\]

see [37] and Appendix, where all relevant notations are introduced, [61,62].

If the Fermi energy sits on the first spectral band it is convenient to use an Intermediate perturbed operator \( l_r \) defined as Schrödinger operator on the whole network with proper matching conditions in all channels except the first one, where the matching boundary condition (50) is replaced by the partial Dirichlet boundary condition, \textit{chopping the first channel off}. For the three-terminal Resonance Quantum Switch we denote by \( E_+ \) the 4-dimensional entrance subspace of open channel, spanned by the first-order eigenfunctions \( e_s \), \( s = 1, 2, 3, 4 \), on the bottom sections \( \gamma_s \), \( s = 1, 2, \ldots \), of the wires of the wires, \( e_1 = \sqrt{\frac{2}{\delta}} \sin \frac{\pi y}{\delta} \), and by \( P_+ \) the corresponding orthogonal projection in \( L_2(\Gamma) \). Then denoting the sum of the bottom sections \( \gamma_s \) by \( \cup \gamma_s = \Gamma \) we present the partial \textit{chopping-off} boundary condition as

\[
P_+ u \big|_\Gamma = 0, \tag{21}
\]

both for the functions from the domain of the corresponding split operator in the wire and in the well. The partial matching condition in all upper (closed) channels with the entrance subspace \( E_- \) and the corresponding complementary projection \( P_- = I_\Gamma \ominus P_+ \) in \( L_2(\Gamma) \) is taken in form:

\[
P_- [u - u_0] \big|_\Gamma = 0, \quad P_- \left[ \frac{1}{m} \frac{\partial u}{\partial n} - \frac{1}{m_0} \frac{\partial u_0}{\partial n} \right] \big|_\Gamma = 0. \tag{22}
\]

The split operator \( l_r \) defined by the above differential expressions [19,20] and the boundary conditions [21,22] can be presented as an orthogonal sum of the trivial part: the one-dimensional Schrödinger operators \( l_s \), \( s = 1, 2, 3, 4 \):

\[
l_s = - \frac{1}{m} \frac{d^2 u}{dx^2} = \frac{1}{m_0} \lambda u_s.
\]
on the open channels with zero boundary conditions at the bottom sections, and the non-trivial part $l_0^r$ defined in the orthogonal complement in Hilbert space of all square-integrable functions on the network $l^r = \sum_{r=1}^4 l_r^r \oplus l_0^r$.

We will use for the intermediate operator the geometrical inscription and the geometrical spectral parameter $\lambda = p^2$ introduced in the previous section. Then the continuous spectrum of the component $l_0^r$ of the intermediate operator on the orthogonal complement of the blocked first channel begins from the second threshold $\frac{m_0}{m_0} \frac{3\pi^2}{3p^2}$. Later we will reveal a special role played by the the eigenvalues $\lambda^r_0$ of $l_0^r$ sitting on the first spectral band $0 < \lambda < \frac{3\pi^2}{3p^2}$.

The intermediate scattering problem may be convert into the original scattering problem via replacement of the partial zero condition (21) in the first channel by the corresponding partial matching condition:

$$P_+ [u - u_0] \bigg|_{l_0^r} = 0, \quad P_+ \left[ \frac{1}{m^2} \frac{\partial u}{\partial n} - \frac{1}{m_0} \frac{\partial u_0}{\partial n} \right] \bigg|_{l_0^r} = 0.$$  \hspace{1cm} (23)

The perturbation caused by this one-dimensional change of the boundary condition (21) to (23) transforms the separated branch of continuous spectrum in the split first channel $0 < \lambda < \infty$ into the branch of continuous spectrum of the original spectral problem. The corresponding scattered waves are combined of Jost solutions $f_{\pm} = e^{\pm i \sqrt{\frac{m_0}{m_0} px}}$, $x > 0$, of the equation \[15\] with compactly-supported potential $[V_l(x) - V_{\infty}] = 0$, $x > 0$ and $[V_l(x) - V_{\infty}] = H^2 - \frac{m_0}{2m_0}$, $-1 < x < 0$:

$$-\frac{d^2 u_1}{dx^2} + \frac{2m^2}{k^2} (V_l(x) - V_{\infty}) u_1 = \frac{m^2}{m_0} p^2 u_1,$$

$$u_1(x) = e^{-i \sqrt{\frac{m_0}{m_0} px} x + e^{i \sqrt{\frac{m_0}{m_0} px} x} S_1 e},$$ \hspace{1cm} (24)

for $l = 1$, $x > 0$, (on the open channel), with any vector $e \in E_s$, accomplished with exponentially decreasing components in upper channels $l > 1$:

$$u_l(x) = e^{i \sqrt{\frac{m_0}{m_0} \left( \frac{m_0}{m_0} + \frac{m_0}{m_0} \right) p^2 x}} S_l e, \quad x > 0, \quad l > 1.$$

Here $S_l$ - the Scattering Matrix - and the amplitudes $S_l$, $l > 1$, in upper channels are defined from the matching condition \[24\] of $u_1$ to the solutions of the corresponding homogeneous equation inside the well.

### 3.4 Scattering matrix

In standard techniques one usually matches the solution of the Schrödinger equation in the domain with the solutions in all (open and closed) channels in the wires. We suggest, see Appendix, sub-section 10.2, a partial matching technique, which requires matching of solutions of the homogeneous intermediate equations with the solutions in open channels of the wires only, thus eliminating infinite algebraic system. Mathematical convenience of this approach, see \[21\] and Appendix below, consists in eliminating of unbounded operators, which are replaced in our approach by finite matrices. Using the partial matching approach based on the intermediate operator gives the following explicit formula for the scattering matrix in case when the split-gate is present:

$$S(p) = -\frac{i \sqrt{\frac{m_0}{m_0}} \frac{\tan \sqrt{\frac{m_0}{m_0} (H^2 - p^2)}}{\sqrt{H^2 - \frac{m_0}{m_0} p^2} + 1} + 1}{\frac{m^2}{m_0} P_+ \Lambda^r P_+ - P_+ Q^r_0 - i \sqrt{\frac{m_0}{m_0}} \frac{\tan \sqrt{\frac{m_0}{m_0} (H^2 - p^2)}}{\sqrt{m_0 (H^2 - p^2)} + 1}} \frac{m^2}{m_0} P_+ \Lambda^r P_+ - P_+ Q^r_0}.$$  \hspace{1cm} (25)
where

\[ Q_i = -i \sqrt{\frac{m_i}{m_0}} p - \sqrt{\frac{m_i}{m_0}} (H^2 - \mu^2) \tanh \sqrt{\frac{m_i}{m_0}} (H^2 - \mu^2) \]

\[ + i \sqrt{\frac{m_i}{m_0}} \mu \tanh \sqrt{\frac{m_i}{m_0}} (H^2 - \mu^2) \]

+ 1

and \( \Lambda^r \) is the Dirichlet-to-Neumann map (DN-map), see \[22 \square11\], of the intermediate operator \( I^r \), see Appendix. The corresponding formula for the case when the split-gate is absent can be obtained via replacement the width \( I \) of the barrier by zero, \( Q_0 = -i \sqrt{\frac{m_0}{m_0}} p \).

The resonance properties of the Scattering matrix \[25\] may be revealed when substituting the spectral series/integral for the \( \Lambda^r = P_+ \Lambda^r P_+ \)

\[ \Lambda^r = \sum_{\lambda} \frac{P_+ \frac{\partial \phi^r}{\partial n}}{\lambda - \lambda_0} \int_0^{2\pi} \frac{P_+ \frac{\partial \phi^r}{\partial n}}{\lambda - \lambda_0} d\lambda + \int_0^{2\pi} \frac{P_+ \frac{\partial \phi^r}{\partial n}}{\lambda - \lambda_0} d\lambda + \ldots \]

Practically the calculation of the DN-map and the Scattering matrix for low temperatures can be reduced to the calculation of the contribution from the singularities of the DN-map of the intermediate operator sitting on the essential interval of energy, see \[15\]. In the next section we neglect the contribution from the upper branch of the continuous spectrum of the intermediate operator and estimate the contribution to the DN-map (and to the Scattering matrix) from the non-resonance terms, \( \lambda_s \neq \lambda_0 \) by the inverse spacing \( \rho^r(\lambda_0^s) \) on the resonance level \( \lambda = \lambda_0^s \) and some dimensional constant \( C \approx |\text{length}|^{-3} \) introduced in section 2.2:

\[ \| \frac{P_+ \frac{\partial \phi^r}{\partial n}}{\lambda - \lambda_0} \| = O \left( \frac{1}{\rho^r(\lambda_0^s)} \right) \leq \frac{C}{|\lambda_0^s - \lambda_s|} \leq \frac{C}{\rho^r(\lambda_0^s)}. \]

In the next section we will show that the most interesting case corresponds to \( I = 0 \). Then the numerator of the scattering matrix is presented for low temperatures as:

\[ \frac{P_+ \frac{\partial \phi^r}{\partial n}}{\lambda - \lambda_0^s} + O \left( \frac{1}{\rho^r(\lambda_0^s)} \right) + i P_+ \frac{m_i}{m_0} p. \]

Leading terms in the numerator near the resonance eigenvalue \( \lambda_0^r \) of the intermediate operator are the polar term \( \frac{P_+ \frac{\partial \phi^r}{\partial n}}{\lambda - \lambda_0^r} \) and the last term \( i P_+ \frac{m_i}{m_0} p \) containing the effective number \( p \). Both of them are homogeneous functions degree \(-1\) of the space variable. The middle term defining the contribution \( O \left( \frac{1}{\rho^r(\lambda_0^s)} \right) \) from the non-resonance eigenvalues is also a homogeneous operator-function degree \(-1\) and can be neglected if the condition \[21\] is fulfilled. In fact one can also develop the perturbation technique for calculation zeroes of (the numerator) of the Scattering matrix based on the small parameter discovered in sub-section 2.3.

If the conditions \[17 \square15\] are fulfilled, then the contribution to the DN-map from the non-resonance terms and upper branches of the absolutely continuous spectrum can be neglected resulting in the resonance term only:

\[ \Lambda^r(\lambda) \approx \frac{P_+ \frac{\partial \phi^r}{\partial n}}{\lambda - \lambda_0^s}. \]

This gives a convenient “one-pole” approximation for the essential DN-map, \( \mathcal{D} \mathcal{N}^r \), and the corresponding “one-pole approximation” for the Scattering matrix which is used in the next section, see \[22\] below. In the next section we use also the above estimation \[20\] for neglected non-resonance terms.
4 The Life-time of resonances and the speed of switching

4.1 Life-time

The $4 \times 4$ Scattering matrix in the first channel is an analytic matrix-function in complex plane of effective wave-number $p$ and may have zeroes - resonances $\{p_s\}$ in the upper half-plane and complex-conjugate poles in the lower half-plane of the complex plane of $p$. In particular, when the split-gate is absent, the resonances can be found as vector-zeroes of the numerator

$$P_+ \frac{\partial \psi_r^*}{\partial n} \langle P_+ \frac{\partial \psi_r^*}{\partial n} e \rangle \lambda - \lambda_r^0 = 0,$$

with a normalized vector $e \in E_\perp$. Multiplying by the orthogonal projection $P_0 = \langle \phi_0 | \phi_0 \rangle$ onto the “resonance entrance vector” $\phi_0' := P_+ \frac{\partial \psi_r^*}{\partial n} := \phi_0 = \{ \phi_0^1, \phi_0^2, \phi_0^3, \phi_0^4 \}$ we may reduce the equation to the pair of equations

$$\left| \phi_0 \right|^2 \frac{\lambda - \lambda_r^0}{\lambda} + \langle P_0 \left( \frac{1}{\rho} (\lambda_r^0) \right) \rangle e + i \sqrt{\frac{m^1}{m_0}} p e = 0,$$

$$-i \sqrt{\frac{m^1}{m_0}} p (P_+ - P_0) e + (P_+ = P_0) \left( \frac{1}{\rho} (\lambda_r^0) \right) e.$$

The first equation is used to estimate the position of the resonance $p$, see the sub-section 2 below, and the second can be used to estimate the deviation of the corresponding zero-vector $e$ from the direction of the “resonance entrance vector” $e_0 = \left| \phi_0 \right|^{-1} \phi_0$. For given resonance $p$ and the corresponding null-vector $e$ a resonance solution $u_0$ of the Schrödinger equation exists, with exponential asymptotic in the wires:

$$u_0(x) = \{ e^1, e^2, e^3, e^4 \} e^{-i \sqrt{\frac{m^1}{m_0}} p x}.$$

The corresponding solution of the non-stationary Schrödinger equation

$$-i \frac{\hbar}{2m_0} \frac{\partial u}{\partial t} \left( \frac{\hbar^2}{2m_0} \Delta u - V(x) u \right)$$

$$u(x,t) = e^{-i \frac{\hbar}{2m_0} p^2 t} u_0(x) := e^{-i \frac{\hbar}{2m_0} p^2 t} u_0(x)$$

is exponentially decreasing with the decrement $\frac{1}{\tau} = \frac{\hbar}{2m_0} \Im p^2$. The inverse decrement $\tau$ is called the life-time of the resonance. The life-time is defined similarly for split-gate closed, as zeroes of the numerator of the expression

$$\frac{P_+ \partial \psi_r^*}{\partial n} \langle P_+ \frac{\partial \psi_r^*}{\partial n} e \rangle \left( \frac{1}{\rho} (\lambda_r^0) \right) e.$$

Note that for dynamics associated with wave equation, see [29], the life-time is usually measured by the inverse imaginary part of the resonance in the plane $p$ of the wave-numbers.

In this section we will calculate the life-time of the resonance approximately estimating the errors appearing from neglecting of the non-resonance terms, in two cases:

1. In case when equivalent split-gates are constructed on the initial part of each wire.

2. In case when split-gates are absent (or switched off) and the wires are attached straight to the quantum well.
4.2 Split-gates closed

Assume that the barrier formed by the split-gate is 1ev over the Fermi level $E_f$ and the Fermi-level is 1ev over the effective bottom $V_\infty + \frac{h^2}{2m}$, and the width $\delta$ of the wire and the width $l$ of the barrier both are 2 nm. Then, due to

$$\frac{2m_0 (V_1 - E_f)}{h^2} = \frac{1}{3.81} \frac{1}{A^2},$$

(30)

the “effective momentum” in the wire, see (48) and below, is estimated as

$$p = \sqrt{\frac{2m_0 (E_f - V_\infty)}{h^2} - \frac{m_0}{m^l} \frac{\pi^2}{\delta^2}} = 0.372 \frac{1}{A},$$

and the under-barrier decay rate is defined by the decrement:

$$\sqrt{\frac{m^l}{m_0}} (H^2 - p^2) = 0.45 \frac{1}{A}.$$

Then $\sqrt{\frac{m^l}{m_0}} (H^2 - p^2) 1 = 9$ and $\tanh \sqrt{\frac{m^l}{m_0}} (H^2 - p^2) 1 = 1 - 2e^{-18} = 1 - 3.45 \times 10^{-8} = 1 - \varepsilon$. The approximate value of the fraction in the numerator may be estimated now as

$$m_0 \frac{i}{m^l} \sqrt{\frac{m^l}{m_0}} p + \sqrt{\frac{m^l}{m_0}} (H^2 - p^2) \tanh \sqrt{\frac{m^l}{m_0}} (H^2 - p^2) 1 =$$

$$= \frac{i}{m^l} (0.95 \times 0.372 + 0.45 (1 - \varepsilon) \times 0.372 + 0.45 \times \frac{1}{2}) [I - 0.246 \varepsilon + i 0.96 \varepsilon].$$

If the distance from the resonance eigenvalue $E_0 \approx E_f$ to the closest upper (second) threshold $\frac{4\pi^2 \hbar^2}{2m^l \lambda^2}$ is greater than $\kappa T$, then the contribution of the continuous spectrum to the $DN$-map of the intermediate operator may be neglected and the zero of the scattering matrix closest to resonance eigenvalue can be found from the equation

$$\left[ P_+ \frac{\partial \varphi}{\partial n} \right] (P_+ \frac{\partial \varphi}{\partial n}) \frac{1}{\lambda - \lambda_0^s} e + \sum_{s \neq 0} P_+ \frac{\partial \varphi}{\partial n} (P_+ \frac{\partial \varphi}{\partial n}) \frac{1}{\lambda - \lambda_0^s} e - m_0 \frac{\partial Q}{\partial n} e = 0.$$

(31)

Here $\varphi^s$ are the normalized eigenfunctions of the Intermediate operator $l'$ which correspond to the eigenvalues on the essential interval of energy. We pass to the non-dimensional coordinates $\xi = R^{-1} x$, assuming that the radius of the well $\Omega$ is 250A. We will use also the non-dimensional spectral parameter: $\lambda = \lambda R^2$ and spacing $\hat{\rho} = \rho R^2$. Then based on the crude estimate of the contribution to $DN$-map from the neighboring (non-resonance) eigenvalues by the input from the closest neighbor:

$$\| \sum_{s \neq 0} P_+ \frac{\partial \varphi^s}{\partial n} (P_+ \frac{\partial \varphi^s}{\partial n}) \frac{1}{\lambda - \lambda_0^s} e \| \leq R^{-1} O \left( \frac{1}{\rho_0^2} \right),$$

we may estimate the one-pole approximation for the non-dimensional $DN$-map $\hat{\Lambda}'$ near to the (non-dimensional) resonance:

$$\hat{\Lambda}' = R^{-1} \hat{\Lambda}^{1,r} = R^{-1} \frac{\hat{\varphi}_0}{\hat{\lambda} - \lambda_0} + R^{-1} O \left( \frac{1}{\hat{\rho}(\lambda_0^s)} \right) =$$

$$R^{-1} \left[ \frac{\hat{\varphi}_0}{\hat{\lambda} - \lambda_0} + O \left( \frac{1}{\hat{\rho}(\lambda_0^s)} \right) \right].$$
For eigenfunctions corresponding to the neighboring eigenvalues we have $|\hat{\phi}_s|^2 \approx 10$, $\hat{\rho}\left(\hat{\lambda}_0^r\right) \approx 2.3$, hence the contribution from the corresponding terms to the DN-map may be estimated based on $\hat{C} < leq 10$ approximately as $R^{-1}\frac{\hat{\rho}}{2} = 4.3/R$. We will use for this quantity the notation $R^{-1}O(4.3)$. Then the equation for zeroes or the Scattering matrix (in non-dimensional scale) may be presented due to $R = 250A$ as:

$$0 = \frac{|\hat{\phi}|^2}{\lambda - \hat{\lambda}_0^r} + O(4.3) + \frac{250}{2} [0.764 + i0.96\epsilon] = \frac{|\hat{\phi}|^2}{\lambda - \hat{\lambda}_0^r} + 95.5 + O(4.3) + i120\epsilon.$$

Then, noticing that $|O(4.3)| << 95.5$, we may neglect the contribution to DN-map from the neighboring non-resonance eigenvalues and obtain the (approximate) position of the zero of the Scattering matrix $\hat{\lambda}^r$ near to the resonance eigenvalue $\hat{\lambda}_0^r$ of the intermediate operator just from the one-pole approximation of DN-map:

$$\hat{\lambda} \approx \hat{\lambda}_0^r - 0.11 + 0.14i\epsilon$$

Hence due to $\epsilon = 2e^{-18} = 10^{-8} 3.45$ the imaginary part of the non-dimensional resonance is $10^{-8} 0.48$. The life-time may be calculated now as

$$\tau = \frac{2m_0}{h} \frac{R^2}{0.48 10^{-8}}$$

with $R^2 = 6.25 10^{-12}cm^2$:

$$\tau = 7.6 10^{-3}sec.$$ This is the speed of the transition process with the split-gate closed.

### 4.3 Split-gates open

Consider the case when the barriers at the entrances to the wires are absent, $l = 0$, or the split-gate open. In this case the equation for resonances may be presented as

$$\left\{ R^{-1} \left[ \hat{\phi}_0 \langle \hat{\phi}_0 | + O \left( \frac{1}{\hat{\rho}(\hat{\lambda}_0^r)} \right) \right] + i\sqrt{\frac{m_0}{m_0}} \hat{p} \right\} e = 0,$$

or, in non-dimensional form:

$$0 = \frac{|\hat{\phi}|^2}{\lambda - \hat{\lambda}_0^r} + O(4.3) + i\sqrt{0.9} \times 250 \times 0.372.$$ Again, we see that the contribution to DN-map from the neighboring non-resonance eigenvalues is dominated by the main term: $O(4.3) << \sqrt{0.9} 250 0.372 = 88$. Then the non-dimensional resonance may be calculated from the one-pole approximation of DN-map as

$$\hat{\lambda} = \hat{\lambda}_0^r - \frac{|\hat{\phi}|^2}{4.3 + 88.2i} = \hat{\lambda}_0^r - 5.5 10^{-3} + i 0.11,$$

and the life-time of the resonance is found as

$$\tau \approx 10^{-11}sec = 10 \pi s.$$ The life-time depends quadratically of the radius of the well, other words, it is quadrupled if the radius of the quantum well is doubled. Vice versa, for the quantum well radius 100 $A$ the life-time with equivalent other parameters is $\tau \approx 2\pi s$. 

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4.4 One-pole approximation of the Scattering matrix

In both cases 4.2 and 4.3 we neglected the contribution to DN-map from the non-resonance eigenvalues, using actually the one-pole approximation for expressions staying in the numerator and denominator of the Scattering matrix taking into account the leading terms of the DN-map only. Consider now the expression for the Scattering matrix combined of the leading terms only. Then, in the second case, we obtain the following “one-pole approximation” \( S_0(\lambda) \) of the Scattering matrix on the essential interval of energy, \( \lambda = \bar{p}^2 \) :

\[
S(\lambda) \approx -\frac{P_+ \frac{\partial \varphi^r}{\partial n}}{\lambda - \lambda_0} + i \sqrt{\frac{m^2}{m_0}} pI = S(\lambda).
\]  

(32)

Note that the zeroes of the function \( S(\lambda) \) can be found from an elementary algebraic equation. The deviation of them from zeroes of the Scattering matrix can be estimated rigorously based on the estimate for the non-resonance terms and the operator version of Rouche theorem, see [21]. One can use the one-pole approximation (32) of the Scattering matrix for approximate description of the electron’s transport across the quantum well, if the conditions (10,9) are fulfilled.

5 Switching Phenomenon

5.1 Shape of the resonance eigenfunction

One can see from the last formula (32) in previous section that the transmission from the input-wire \( \Omega_1 \) to the terminal \( \Omega_s \) is blocked, if for given magnitude \( E \) of the constant electric field in the basic domain \( \Omega_0 \) the projection of the normal derivative of the resonance eigenfunction \( \varphi^r_0 \) of the intermediate operator onto the corresponding eigenvector on the cross-section of the open channel \( e^*_1 = \sqrt{\frac{8}{\pi}} \sin \frac{\pi \bar{y}}{s} \) vanishes. Practically this condition is fulfilled if a zero of the normal derivative of the resonance eigenfunction \( \varphi^r_0 \) in the basic domain sits at the center \( a_s \) of the bottom section of the wire \( \Omega_s \). This means that the single-mode transmission of an electron across the quantum well is implemented via excitation of the resonance mode \( \varphi^r_0 \) inside the quantum well \( \Omega_0 \) and the transmission coefficients are defined by the local properties of the resonance eigenfunction of the intermediate operator in the domain near to the bottom sections \( \Gamma_s \) of the wires.

It was noticed in [32,33] that the design of the network and the magnitude of the constant field inside the basic domain may be selected such that the zeroes of the normal derivative of the resonance eigenfunction are sitting on the entrances of two wires simultaneously, leaving the input wire and one of terminals non-blocked. One can show, that the resonance entrance vector \( \hat{\varphi}_0 = P_+ \frac{\partial \varphi^r_0}{\partial n} \) produced from the resonance eigenfunction of the intermediate operator (with the first channel “chopped off”) coincides with the corresponding portion \( \hat{\varphi}_0 = P_+ \frac{\partial \varphi^r_0}{\partial n} \) of the eigenfunction \( \varphi_0 \) of the Dirichlet problem in the quantum well, see Appendix, subsection 9.3. In this section we do not distinguish resonance entrance vectors obtained from eigenfunctions of the Intermediate operator and one of the Dirichlet problem on the well. Our calculations with Dirichlet problem in [33] show that: if the non-dimensional amplitude \( e = \frac{2mE^2}{\hbar} \) of the macroscopic electric field \( E \) inside the quantum well \( \Omega_0 \) is chosen as 18.86, then the eigenfunction \( \hat{\varphi}_0 \) corresponding to the non-dimensional resonance eigenvalue \( \lambda_0 = 14.62 \) inside the well has a single line of zeroes inside the well and zeroes of it’s normal derivative sit on the unit circle at the points forming angles \( \pm \frac{\pi}{3} \) with the direction of the unit vector \( \nu \). This eigenfunction is even with respect to reflection in the line spanned by the vector \( \nu \). The nearest eigenvalues of the even series of eigenfunctions sit at \( \bar{\lambda} = 2.10, 25.82 \). The nearest eigenvalues of the odd series of eigenfunctions are 5.78, 12.32, 25.99.

5.2 Transmission coefficients

The resonance entrance vector \( \hat{\varphi}_0 \) computed with use of the normalized eigenfunction \( \hat{\varphi}_0 \) of the non-dimensional Intermediate operator or Schrödinger operator on the well with the potential defined by the
vector $\nu$ directed to the point $a_1$ (to the entrance of the input wire) has the components $[10]:$

$$\hat{\phi}_0 = (1, 0.1, 3, 0.1),$$

(33)

hence $||\hat{\phi}_0||^2 = C \approx 10$. Then the transmission coefficients may be calculated from the one-pole approximation $[32]$ as:

$$|T_{12}| = |T_{14}| = 0.02, |T_{13}| = 0.6.$$

Really, using the one-pole approximation for the Scattering matrix presented as a function of the geometric spectral parameter $\lambda = \bar{p}$ near to resonance $\lambda_0$:

$$S(\lambda) \approx -\frac{\hat{\phi}_0}{\lambda - \lambda_0} + ip\sqrt{\frac{m^2}{m_0}} I - 2 \hat{\phi}_0 \hat{\phi}_0^\dagger \frac{1}{1 + i \sqrt{\frac{m}{m_0}} \rho(\lambda - \lambda)_0^2}.$$

which gives the transmission coefficients as non-diagonal elements of the Scattering matrix and implies the announced result at $\lambda = \lambda_0$. This permits to calculate the ratio of amplitudes of the signal in closed and open wires as $1 : 30$ and calculate the conductance from the input wire to the open wire $\Omega_3$ just from the Landauer formula, see $[28]$, since other wires $\Omega_{2,4}$ are closed:

$$\sigma_{13} \approx \frac{e^2}{h} \frac{T_{13}^2}{1 - T_{13}} = \frac{e^2}{h} \frac{0.36}{0.64}.$$

(34)

This result holds for zero absolute temperature and for spin-polarized electrons. For non-polarized electrons the result should be doubled. The transmission coefficient at the resonance energy for non-zero absolute temperature should be obtained via averaging over the Fermi-distribution on the essential interval of energy $(E_F - \kappa T, E_F + \kappa T)$, similarly to $[57]$, and may give a result close to the previous one $[31]$, or close to zero in two limit cases

$$\kappa T << \frac{\hbar}{\tau} \text{ or } \kappa T >> \frac{\hbar}{\tau}$$

(35)

respectively.

The above formulae show that in certain range of temperatures the transmission is proportional to the product of components $(\frac{\partial \varphi_0}{\partial a_1}, e_s)$ of the resonance entrance vector on the bottom sections of the corresponding wires, in complete agreement with the basic observation in $[19]$ quoted in the Introduction. Similar fact for the switch based on the quantum well with Neumann boundary conditions was noticed in $[32]$. An analog of it remains true for the scattering on the quantum ring, see $[10]$.

One may obviously construct the dyadic(one input and two terminals) Resonance Quantum Switch (RQS-2) based on the above observation concerning the transmission coefficients. Triadic (three-terminal) switch (RQS-3) can be constructed when selecting the magnitude of the governing electric field as proposed in $[32, 33]$ with the resonance eigenfunction possessing two zeroes of the normal derivative dividing the boundary of the well in ratio $1 : 2$. Taking into account that the zeroes move on the boundary of the well together with rotation of the vector $\nu$, one can see that the directing the vector opposite to the contact point $a_s$ shifts the zeroes of the normal derivative to the complementary contact points, thus blocking the complementary wires on the essential interval of energy.

### 6 Working point of the triadic Resonance Quantum Switch

The working point $R, \mathcal{E}, V_0$ of the triadic Resonance Quantum Switch (RQS) is defined by the position of the resonance energy level of the intermediate operator (or the Schrödinger operator inside the well) closest to the Fermi level on the wires, the above “geometric” property of the resonance eigenfunction $\varphi_0$, the single-mode condition on the wires, and the temperature. It was noticed above that the position of the working point of the triadic switch RQS-3 can’t be defined experimentally just by the straightforward scanning on one of parameters with other parameters fixed at random, since the probability of proper choice of remaining parameters is zero, being proportional to the zero-measure of a point on a $2 - d$ plane.
Consider the three-terminal Resonance Quantum Switch (RQS) constructed in form of a circular quantum well \( \Omega_0 \) with four quantum wires \( \Omega_s \), \( s = 1, 2, 3, 4 \), attached to it at the contact points \( a_1, a_2, a_3, a_4 \), selected as suggested above, such that the entrances to terminals \( a_2, a_3, a_4 \) divide the boundary of the circular well into three equal parts. Assuming that the spectral properties of the non-dimensional Schrödinger operator are already defined to fulfill the above geometric condition on the resonance eigenfunction, we choose the working point of the switch in dependence of desired temperature. Consider first the non-dimensional Schrödinger equation in the unit disc \(|\xi| < 1\) with Dirichlet boundary conditions at the boundary. It was obtained, see \( 10 \), from the original equation by scaling \( x = R \xi \) in the geometrical form \( 19 \) of the Schrödinger equation for the values of energy on the first spectral band:

\[
- \triangle \xi u + \frac{2m_0 e \mathcal{E} R^3}{\hbar^2} (\xi, \nu) u + \frac{2m_0 R^2}{\hbar^2} \left[ V_0 - V_\infty - \frac{\hbar^2}{2m_\perp} \left( \frac{\pi}{\delta} \right)^2 \right] u = \hat{p}^2 = \hat{\lambda} u. \tag{36}
\]

Here \( \hat{\lambda} = \hat{p}^2 = R^2 \hat{p}^2 = R^2 \lambda \) is the non-dimensional spectral parameter, \( \mathcal{E} \) is the magnitude of the selected electric field, \( V_0 \) is the additional constant “background” potential on the well \( \Omega_0 \), and \( V_\infty \) is the potential in quantum wires. The unit vector \( \nu \) defines the direction of the electric field, \( e \) is the electron charge and \( R \) is the radius of the circular well. Selecting \( e = -\frac{2m_0 e \mathcal{E} R^3}{\hbar^2} = 18.86 \), where \( e \) is now the absolute value of the electron’s charge, one may see that the eigenfunction of the equation

\[
- \triangle \xi u - e (\xi, \nu) u = \hat{\lambda} u = \hat{p}^2 u, \tag{37}
\]

corresponding to the second lowest eigenvalue 14.62

\[
\hat{\lambda}_0 = \hat{\lambda}_0 - 2m_0 \frac{R^2}{\hbar^2} \left[ V_0 - V_\infty - \frac{\hbar^2}{2m_\perp} \left( \frac{\pi}{\delta} \right)^2 \right] = \hat{\lambda}_0 - V_0
\]

of the even series has proper positions of zeroes of the normal derivative on the boundary of the well.

The minimal distance \( \hat{\rho}_0 \) of \( \hat{\lambda}_0 = 14.62 \) from the nearest non-dimensional eigenvalue 12.32 (non-dimensional spacing) is 2.3. The working regime of the switch will be stable if the bound states in the well corresponding to the neighboring eigenvalues will not be excited at the temperature \( T \):

\[
\kappa T \frac{2m_0 R^2}{\hbar^2} \leq \hat{\rho}_0 = \frac{2}{2}. \tag{38}
\]

This condition may be formulated in terms of the scaled temperature \( \hat{T} = \frac{2m_0 R^2 T}{\hbar^2} \) as

\[
\kappa \hat{T} < \frac{\hat{\rho}_0}{2} = \frac{2.3}{2}. \tag{39}
\]

The temperature which fulfills the above condition we may call low temperature, for given device. If the radius \( R \) of the corresponding quantum well is small enough, then the condition \( 39 \) can be fulfilled for some (absolutely) high temperature, which corresponds to the relative low scaled temperature. For instance, the effective mass \( m_0 \) of electron in the well (for a narrow-gap semiconductor) may be small, see \( 14, 50 \), then even the room-temperature may be “low” enough after proper scaling.

Importance of developing technologies of producing devices of small size with rather high potential barriers is systematically underlined when discussing the prospects of nano-electronics, see for instance \( 14 \). Use of narrow-gap materials may open a way to room-temperature devices of reasonably large dimensions.

Assume that the Fermi level sits in the middle of the first spectral band. Then we obtain the estimate of the radius \( R \) of the domain and the width of the wires from \( 38 \) as:

\[
R^2 \leq \frac{2.3 \hbar^2}{2 \kappa T \delta m_0}, \quad \delta < \frac{R}{\frac{2}{2}}. \tag{40}
\]

For the fixed radius \( R \), the shift potential \( V_0 \) on the well \( \Omega_0 \) may be defined from the condition

\[
\frac{2m_0 R^2 |E_\infty - V_0 - V_\infty| - \frac{\hbar^2}{2m_\perp} \frac{\pi^2}{3^2}}{\hbar^2} = \hat{\lambda}_0.
\]
For instance, if we choose the radius $R$ of the domain as $R^2 = \frac{\hat{\rho}_0 \hbar^2}{4m_0 \kappa T}$ and $\delta = R/2$, we obtain the value of the shift potential on the well:

$$V_0 = E_f - V_{\infty} - \frac{\hbar^2 \pi^2}{2m_0 \delta^2} - \frac{\hbar^2 \hat{\lambda}_0}{2m_0 R^2} = \kappa T \left( 60 \frac{m_0}{m^*} - 13 \right)$$

Finally, the electric field $E$ may be found from the condition

$$e = 18.86 = e\frac{2m_0 R^3}{\hbar},$$

where $e$ is the absolute value of the electron charge. Hence for the value of $R$ selected as above we have:

$$e\kappa T R = 18.86 \frac{\hbar^2}{2m_0 R^2} \approx 17\kappa T.$$}

The electric field obtained from this condition is strong enough to guarantee proper shape of the resonance wave-function, but not yet destructive for semiconductors listed below.

One can see from the above calculations that the switch will work even at room temperature if the radius $R$ of the quantum well is small enough and the geometric details are exact.

Calculation of the radius of the quantum well (in Angstroms) for different materials gives the following results, [30]:

| Material      | $m/m_0$ | $R_{300K}$ | $R_{77K}$ |
|---------------|---------|------------|-----------|
| Cd$_{0.15}$Hg$_{0.85}$Te | 0.0069  | 160        | 310       |
| InSb          | 0.013   | 110        | 230       |
| InAs          | 0.023   | 90         | 170       |
| GaAs          | 0.067   | 50         | 100       |
| Si            | 0.8     | 10         | 25        |

The De-Broglie wavelengths of that materials are, correspondingly, for Nitrogen temperature, 1300A, 970A, 730A, 430, 110A. To obtain the above data we use in the formula (40) instead of $m_0$ the average value of the effective mass $m$ inside the quantum well. For Si the local values may essentially deviate from the average value 0.8, depending on local positions of valleys. Note that the Fermi surface of the narrow-gap material Cd$_{0.15}$Hg$_{0.85}$Te in momentum space is spherically symmetric, hence $m^* = m^\parallel$. This important fact permits to simplify the above formulae for the transmission coefficients.

### 7 Solvable model

The above one-pole approximation [32] and even similar “few-poles” approximation [1] of the Scattering matrix of the switch:

$$\frac{ipI + \Lambda^\tau}{ipI - \Lambda^\tau} = S_\tau(\lambda),$$

with rational essential DN-map of the intermediate operator presented as a function of the geometric spectral parameter $\lambda = p$:

$$\Lambda^\tau(\lambda) = \sum_{\lambda_i \in \Delta_\tau} \frac{P_+ \frac{\partial \varphi^\tau}{\partial \eta}(P_+ \frac{\partial \varphi^\tau}{\partial \eta})}{\lambda - \lambda_i}$$

(41)

can be interpreted as a Scattering matrix of some solvable model. We sketch here the construction of the solvable model of the switch, or, more generally, of a multiple splitting of the quantum wire, based on operator extension procedure, see the general outline of extension theory with applications to general quantum solvable models in [3, 43, 4], and especially to modelling of Quantum networks in [34].
We will construct the model based on “zero-range potential with inner structure” as an extension of an orthogonal sum of one-dimensional matrix Schrödinger with zero potential on the space $L_i(R_+, E_+)$ of open channels

$$l_+ u = -\frac{d^2 u}{dx^2} = \frac{m}{m_0} \lambda u,$$

with respect to the non-dimensional coordinates \( \hat{x} = x \) and non-dimensional spectral parameter \( \hat{\lambda} = \lambda = \frac{p^2}{\hbar^2} \), and some finite-dimensional hermitian Hamiltonian \( H_0 \) of inner degrees of freedom (“inner Hamiltonian”), which defines the “inner structure” of the model. The integration by parts on functions with no boundary conditions at the contact point \( x = 0 \) gives the boundary form of the exterior part

$$\mathcal{J}_o(\psi, \varphi) = \langle l_+ \psi, \varphi \rangle - \langle \psi, l_+ \varphi \rangle = \langle \psi', \varphi \rangle - \langle \varphi', \psi \rangle \quad (42)$$

where \( \psi = \psi(0) = (\psi_1(0), \psi_2(0), \psi_3(0)) \) and the derivatives \( \psi' \) at the node \( x = 0 \) are taken in the outgoing direction. The corresponding boundary form for properly modified inner Hamiltonian \( H_0 \) can be obtained via abstract integration by parts, see [43]:

$$\mathcal{J}_i(\psi^{in}, \varphi^{in}) = (\xi^i_+, \xi^i_-) - (\xi^i_-, \xi^i_+).$$

The sum of boundary forms \( \mathcal{J}_o(\psi, \varphi) + \mathcal{J}_i(\psi^{in}, \varphi^{in}) \) vanishes on the Lagrangian plane which can be defined by the boundary condition with some hermitian matrix \( B \):

$$\begin{pmatrix} \psi' \\ -\xi^i_+ \end{pmatrix} = \begin{pmatrix} \beta_{00} & \beta_{01} \\ \beta_{10} & 0 \end{pmatrix} \begin{pmatrix} \psi \\ -\xi^i_- \end{pmatrix}, \quad (43)$$

where \( \beta_{01} = (\beta^1_{01}, \beta^2_{01}, \ldots) \) is the operator connecting the inner deficiency subspace \( N_i \) of the modified inner Hamiltonian with the entrance subspace \( E_+ \) of the open channels. This boundary condition defines a self-adjoint operator \( \mathcal{L} \) which may serve a solvable model of the Schrödinger operator \( \mathcal{L} \) on the quantum switch, if we select the parameters \( H_0 \) and \( B \) to fulfill certain conditions for given Fermi level \( E_F = \frac{\hbar^2}{2m_0} \lambda_F + V_\infty + \frac{e^2}{2m_1 \hbar^2} \) from the first spectral band , \( 0 < \lambda_F < \frac{m_0}{m_1} \frac{3\pi^2 R^2}{\delta} \) in the wires and given temperature.

$$\lambda_F - \frac{2m_0 R^2}{\hbar^2} \kappa T < \lambda_s < \lambda_F + \frac{2m_0 R^2}{\hbar^2} \kappa T.$$ 

We assume that the few-pole approximation \( S_F \) is defined by the corresponding essential DN-map which is a sum of few terms with poles at the positive eigenvalues \( \lambda_s, \ s = 0, 1, 2, \ldots n_F \) in the corresponding essential interval \( \Delta_F = \left( \lambda_F - \frac{2m_0 R^2}{\hbar^2} \kappa T, \lambda_F + \frac{2m_0 R^2}{\hbar^2} \kappa T \right) \) of the spectral parameter.

Scattering matrix of the model can be calculated in explicit form based on the boundary condition (43) connecting the boundary data \( \xi^i_+ \) of the inner component of the wave function of the switch. Using the equation \( \xi^i_- = -\mathcal{M} \xi^i_+ \) derived with use of the Krein’s Q-function \( \mathcal{M}(\lambda) = P_{N_i} \frac{I + \lambda H}{H - \lambda \mathcal{M}} P_{N_i} \), see [43], we can eliminate the boundary data \( \xi^i_+ \) of the inner component of the wave function

$$\xi^i_+ = -\beta_{10} [(I + S)e + se]$$

and obtain an expression for \( S \) from the matching conditions [43] of the inner component of the wave-function of the model with the Scattering Ansatz in the open channels

$$\psi(x) = e^{-ipx} e + e^{ipx} S(\lambda) e,$$

where \( e \in E_+ \) and \( S(\lambda) \). The Scattering matrix of the model is found as:

$$S(\lambda) = \frac{ip + [\beta_{00} - \beta_{01} \mathcal{M} \beta_{10}]}{ip - [\beta_{00} - \beta_{01} \mathcal{M} \beta_{10}]}.$$
Our aim is: to define the parameters $B, H$ of the model such that the above Scattering matrix $S$ coincides with the essential Scattering matrix $S_\tau(\lambda)$ of the switch.

Denote by $Q_t$ the spectral projection onto the eigen-space of $H$ corresponding to the eigenvalue $\lambda_t$ framed by projections onto the deficiency subspace $N_i$

$$Q_t = P_i e_{\lambda_t}\langle P_i e_{\lambda_t}.$$  

Then the expression in the numerator of the model Scattering matrix takes the form:

$$[\beta_{00} - \beta_{01} M \beta_{10}] = \left[ \beta_{00} + \sum_i \lambda_i \beta_{01} Q_i \beta_{10} \right] + \sum_t \frac{1 + \lambda_t}{\lambda_t - \lambda_0} \beta_{01} Q_t \beta_{10}. \quad (44)$$

We will define the boundary parameters later, but once they are defined, we choose $\beta_{00}$ such that the first summand in (44) vanishes: $\beta_{00} + \sum_i \lambda_i \beta_{01} Q_i \beta_{10} = 0$. This condition guarantees correct behavior of the model Scattering matrix for large $\lambda$ which is typical for real Scattering matrices and for above few-pole approximations (41) of the DN-map $\Lambda^r_T$. Compare now the remaining summand $\sum_t \frac{1 + \lambda_t^2}{\lambda_t - \lambda} \lambda_t \beta_{01} Q_t \beta_{10}$ of the Krein- function with the essential part $\Lambda_T^\tau$ of the DN-map of the intermediate operator which is presented as a sum of polar terms

$$- \sum_{\lambda_t \in \Delta_T} P \frac{\beta_{t \tau}}{\lambda_t - \lambda}.$$

From (44, 45) we see, that the eigenvalues $\lambda_s$ of the model inner Hamiltonian should coincide with essential eigenvalues $\lambda_s$ of the intermediate operator. The boundary parameters and the deficiency subspaces of the model should be selected such that all residues of the Krein function coincide with residues of the essential part $\Lambda_T^\tau$ of the DN-map of the intermediate operator. Then the model Scattering matrix takes the form:

$$S(k) = \frac{ipI - \sum \frac{1 + \lambda_t^2}{\lambda_t - \lambda_0} \lambda_t \beta_{01} Q_t \beta_{10}}{ipI + \sum \frac{1 + \lambda_t^2}{\lambda_t - \lambda_0} \lambda_t \beta_{01} Q_t \beta_{10}}, \quad (46)$$

with $I = I_+$ equal to the unit operator in $E_+$. In case when only one resonance eigen-value $\lambda_0$ of the intermediate operator sits on the admissible interval of energy, the model Scattering matrix

$$S(k) = \frac{ipI - \frac{1 + \lambda_0^2}{\lambda_0 - \lambda_0} \lambda_0 \beta_{01} Q_0 \beta_{10}}{ipI + \frac{1 + \lambda_0^2}{\lambda_0 - \lambda_0} \lambda_0 \beta_{01} Q_0 \beta_{10}}, \quad (47)$$

is a one-pole approximation of the Scattering matrix of the network.

## 8 Conclusion

Working parameters of the switch were estimated based on one-pole approximation of the Scattering matrix which coincides with an exact Scattering matrix of some solvable model of the Quantum Switch. The developed approach, based on the observation from [19] quoted above in Introduction, can be used not only for design of devices aimed to manipulation the current across quantum dots with constant electric field, but also to corresponding non-stationary problems, like Quantum pumping, see [35] and even for spin-filtering [51], based on Rashba spin-orbital Hamiltonian. [45, 13]. On the other hand, taking into account details of the shape of the wave-function encoded in the corresponding Dirichlet-to-Neumann map, rather than just in the “overlapping integrals”, may help understanding functioning of molecular mechanisms. In particular, it can be used for optimization of construction of molecular mechanisms and estimation of admissible errors in design and choice of physical parameters of them.

Note that the general program of replacement of the partial Schrödinger equation on complex quasi-one-dimensional structures with properly chosen solvable models of Schrödinger operators is being developed already in a series of papers and books [29, 31, 32, 33, 36, 49, 25, 4, 27, 21, 26] and in our papers [10, 32, 28] where solvable models of switches were considered.
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10 Appendix

In this section we review the techniques of matching solutions of the Schrödinger equation in composite domains and, in particular, derive the exact (25) and approximate (32) expressions for the Scattering matrix used above. Mathematical nature of some statements presented in this section forces us to choose for them a non-dimensional form. We begin with descriptions of these forms, both in case when the split - gates are present on the initial part of the wires (−1, 0), or absent, l = 0.

In both cases the Schrödinger equation on the wires admits separation of variables when presenting the solution as an expansion over eigenfunctions of the cross-sections $e_l(y) = \sqrt{\frac{2}{\delta}} \sin \frac{\pi l}{\delta}y$, $0 < y < \delta$, $u = \sum_{l=1}^{\infty} u_l(x) e_l(y)$. Denoting by $V_1(x)$ the potential on the wire

$$V_1(x) = \begin{cases} V_{\text{barrier}} + V_\infty, & \text{if } (-1 < x < 0) \\ V_\infty, & \text{if } (0 < x < \infty), \end{cases}$$

we may present the equations for the amplitudes $u_l$, $l = 1, 2, \ldots$ as

$$-\frac{d^2 u_l}{dx^2} + \frac{2m_l}{\hbar^2} [V_1(x) - V_\infty] u_l - \frac{m_l}{m_0} \frac{\pi^2 (l^2 - 1)}{\delta^2} u_l = \frac{m_l}{m_0} u_l, \quad l = 1, 2, \ldots \quad (48)$$

with the spectral parameter $\lambda = p^2 = \frac{2m_0}{\hbar^2} \left[ E - V_\infty - \frac{\hbar^2}{2m_0} \frac{\pi^2}{\delta^2} \right]$. Here $p$ is the “effective wave-number ” in the wires. The function $u = \sum_{l=1}^{\infty} u_l(x) e_l(y)$ should match, on the sum $\Gamma = \cup_s \Gamma_s$ of the bottom sections $\Gamma_s$, $s = 1, 2, \ldots$ of the wires, the corresponding solution $u_0$ of the Schrödinger equation with linear potential on the well. This equation may be presented in geometrical form as

$$\frac{2m_0}{\hbar^2} l u_0 = -\Delta u_0 + \frac{2m_0}{\hbar^2} \left[ \mathcal{E} e(x, \nu) + V_0 - V_\infty - \frac{\hbar^2}{2m_0} \frac{\pi^2}{\delta^2} \right] u_0 =$$
In terms of the spectral parameter $\lambda = p^2$ we can re-write the above equation (49) in geometric form with use of the re-normalized shift potential $V_0 = \frac{2m_0}{\hbar^2} [V_0 - V_\infty - \frac{\hbar^2 \pi^2}{2m^\perp \delta^2}]$ and the re-normalized electric potential $e_\langle x, \nu \rangle := -\frac{2m_0 \hbar}{\hbar} e_\langle x, \nu \rangle$:

$$-\triangle u_0 - e_\langle x, \nu \rangle u_0 + V_0 u_0 = \lambda u_0 = p^2 u_0.$$  

(51)

The Schrödinger equation on the wires reduced to the same spectral parameter takes the form

$$-\frac{d^2 u}{dx^2} - \frac{m^\parallel}{m} \frac{d^2 u}{dy^2} - \frac{m}{m^\perp} \frac{\pi^2}{\delta^2} u + V_s(x) u_s = \frac{m}{m_o} \lambda u_s$$  

(52)

with corresponding effective potential $V_s(x)$ vanishing for $x > 0$.

We assume now that the potential in the wires is constant $V_s(x) = V_\infty$ (the barrier on the initial part of each wire is absent, $l = 0$). As before in sections 1,2 we present the Schrödinger equation in the wires in “geometric form” on the open channel as:

$$-\frac{d^2 u}{dx^2} = \left\{ \frac{2m^\parallel}{m} \left[ E - V_\infty \right] - \frac{m^\parallel}{m^\perp} \left( \frac{\pi^2}{\delta^2} \right) \right\} u := \frac{m^\parallel}{m_o} p^2 u = \frac{m^\parallel}{m_o} \lambda u$$  

(53)

and on the closed channels $l = 2, 3, \ldots$ as

$$-\frac{d^2 u}{dx^2} = -\frac{m^\parallel}{m_0} \left( \frac{l^2 \pi^2}{\delta^2} \right) u := -\frac{m^\parallel}{m_0} \left[ (l^2 - 1) \frac{\pi^2}{\delta^2} - \frac{m_0}{m^\perp} p^2 \right] u_0.$$  

The geometric form of the Schrödinger equation on the quantum well is the same, (51). Introducing the non-dimensional variable $\xi = x/R$ and the non-dimensional coefficients $e = \frac{2m_0 R^2 \hbar^2}{\hbar^2}$, $V_0 = R^2 \left[ \frac{2m_0}{\hbar^2} (V_0 - V_\infty) - \frac{\pi^2}{\delta^2} \frac{m_0}{m^\perp} \right]$ we may present the equations in the open channel of the wires in non-dimensional form:

$$-\frac{d^2 \hat{u}}{d\xi^2} = \frac{m^\parallel}{m_0} \hat{p}^2 \hat{u} = \frac{m^\parallel}{m_0} \hat{\lambda} u$$  

(54)

with the non-dimensional wave-number $\hat{p} = pR$ or non-dimensional spectral parameter $\hat{\lambda}$ in the first channel, and in form

$$-\frac{d^2 \hat{u}}{d\xi^2} + \frac{m^\parallel}{m^\perp} \frac{R^2 \pi^2 (l^2 - 1)}{\delta^2} u = \frac{m^\parallel}{m_0} \hat{p}^2 \hat{u} = \frac{m^\parallel}{m_0} \hat{\lambda} u$$  

(55)

in closed channels. On the quantum well it takes the form:

$$-\triangle \xi \hat{u} - e_\langle \xi, \nu \rangle \hat{u} + \hat{V}_0 \hat{u} = \hat{p}^2 \hat{u},$$  

(56)

with $\hat{V}_0 = R^2 V_0$.

10.2 Dirichlet-to-Neumann Map

**Standard DN-map** Dirichlet-to-Neumann map for the Schrödinger equation in geometric form in a domain $\Omega$ is a map of the boundary values $u_{\Gamma}$ of the solution

$$-\triangle u + Vu = \lambda u, \quad u|_{\partial \Omega_0} = u_{\Gamma}$$

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on the border $\partial \Omega = \Gamma$ of the domain into the boundary values of it’s normal derivative:

$$\Lambda : u_\Gamma \rightarrow \frac{\partial u}{\partial n}|_{\Gamma_{\partial \Omega}}.$$  

In electrodynamics (with $V = 0$) this corresponds to the connection of the potential on the boundary with the normal current. Detailed description of general features of the DN-map and it’s relations to the Scattering Matrix may be found in [52, 41], respectively. We will review here only basic features of the standard DN-map.

Denote by $L_D$ and $L_N$ the self-adjoint operators defined in $L^2(\Omega_0)$ by the above differential expression $Lu = -\Delta u + Vu$ and homogeneous Dirichlet and Neumann boundary conditions respectively. Corresponding Green functions $G_{N,D}(x, y, \lambda)$ and the Poisson kernel $P_{\lambda}(x, s) = -\frac{\partial G_D(x, s, \lambda)}{\partial n_s}$, $s \in \partial \Gamma$, exist if $\lambda$ is not an eigenvalue of the corresponding operator $L_D$ (is “regular”). Solutions of classical boundary problems for operators $L_{N,D}$ may be represented for regular $\lambda$ by the “re-normalized” potentials of densities supported by the boundary $\Gamma_0$. For instance for the Neumann problem

$$Lu = \lambda u, \quad \frac{\partial u}{\partial n}|_\Gamma = \rho$$

with N-regular (regular for Neumann problem) $\lambda$ we obtain the solution as a re-normalized simple-layer potential:

$$u(x) = \int_\Gamma G_N(x, s, \lambda)\rho(s)d\Gamma.$$  \hspace{1cm} (57)  

For the Dirichlet problem with D-regular $\lambda$

$$Lu = \lambda u, \quad u|_\Gamma = u_\Gamma$$

we obtain the solution as a re-normalized double-layer potential:

$$u(x) = \int_\Gamma P_D(x, s, \lambda)u_\Gamma(s)d\Gamma.$$  \hspace{1cm} (58)  

Generally the standard DN-map is represented for regular points $\lambda$ of $L_D$ as a generalized integral operator with a singular kernel:

$$(\Lambda(\lambda)u_\Gamma)(x_\Gamma) = \frac{\partial}{\partial n}|_{x = x_\Gamma} \int_{\partial \Omega} P_D(x, s, \lambda)u_\Gamma(s)d\Gamma$$

and exist as an operator in proper functional classes. In particular for operators defined on $W_2^2(\Omega)$ it acts in proper Sobolev classes, see [31], as:

$${\Lambda(\lambda)} : W_2^{3/2}(\Gamma) \rightarrow W_2^{1/2}(\Gamma)$$

see for instance [52, 41]. One can see from the straightforward integration by parts that the DN-map is an analytic function of the spectral parameter $\lambda$ with a negative imaginary part (for interior problem, with an outer positive normal on the boundary).

The following simple statement, see [41], shows, that the singularities of the kernel of the DN-map $\Lambda_{in}(\lambda)$ in space variable and the poles at the eigenvalues of the inner Dirichlet problem may be in certain sense separated:
**Theorem 10.1** Let us consider the Schrödinger operator \( L_D = -\Delta + q(x) \) in \( L_2(\Omega) \) with real potential \( q \) and homogeneous Dirichlet boundary condition on the smooth boundary \( \Gamma \) of the bounded domain \( \Omega \). Then the DN-map \( \Lambda \) of \( L_D \), defined on the Sobolev class \( W_{2,0}^2 \), satisfying homogeneous Dirichlet boundary conditions on \( \partial\Omega \) has the following representation on the complement of the corresponding spectrum \( \sigma_L \) in complex plane \( \lambda, M > 0 \):

\[
\Lambda(\lambda) = \Lambda(-M) - (\lambda + M)P_M^+ P_M - (\lambda + M)^2 P_M^+ R_\lambda^+ P_M^-,
\]

where \( R_\lambda \) is the resolvent of \( L_D \), and \( P_M \) is the Poisson map of it. The operators

\[
\Lambda(-M), \ (P_M^+ P_M)(x_\Gamma, y_\Gamma)
\]

are bounded in proper Sobolev classes: respectively from \( W_{3/2}^2(\Gamma) \) onto \( W_{1/2}^1(\Gamma) \) and in \( W_{3/2}^2(\Gamma) \), and the operator

\[-(\lambda + M)^2 \ (P_M^+ R_\lambda P_M)(x_\Gamma, y_\Gamma)\]

may be presented by the convergent spectral series

\[
-(\lambda + M)^2 \sum_{\lambda_s \in \sigma_L} \frac{\partial \phi_{\lambda_s}(x_\Gamma)}{\partial n_s} \frac{\partial \phi_{\lambda_s}(y_\Gamma)}{\partial n_s} \frac{1}{(\lambda_s - \lambda)}
\]

and is compact in \( L_2(\Gamma) \).

Note that the last term of the sum (60) presented as (61) reveals an explicit dependence of the standard DN-map of the eigenvalues of the inner Dirichlet problem in \( \Omega_o \). The corresponding formal “spectral expansion” for the kernel of the DN-map

\[
\Lambda(\lambda)(x_\Gamma, y_\Gamma) = \sum_{\lambda_s \in \sigma_L} \frac{\partial \phi_{\lambda_s}(x_\Gamma)}{\partial n_s} \frac{\partial \phi_{\lambda_s}(y_\Gamma)}{\partial n_s} \frac{1}{(\lambda_s - \lambda)}
\]

is divergent.

**Scattering matrix via standard matching** The standard DN-map permits to formalize the procedure of matching solutions of partial differential equation in the composite domain \( \Omega_o \cup \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_4 \) which have a common piece of boundary \( \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4 = \Gamma \).

Denote by \( E_+ \) the 4-dimensional subspace in \( L_2(\gamma) = E \) spanned by the vectors \( e_s^1, s = 1, 2, 3, 4 \). \( E_+ \) plays the role of the “entrance subspace” of open channels in the wires if \( 0 < p^2 < \frac{m_0}{m_+} \left( \frac{4\pi^2}{\delta^2} \right) \). The orthogonal complement of it \( E \cap E_+ = E_- \) is the entrance subspace of closed channels. On the first spectral band

\[
0 \leq \lambda \leq \frac{m_0}{m_+} \frac{3\pi^2}{\delta^2}
\]

there are two bounded exponential modes of the first order based on the cross-section eigenfunction \( e_s^1 = \sqrt{2} \sin \frac{\pi y}{\delta} \) in the wire \( \Omega_s \) with exponentials defined by \( p \):

\[
f_s^+_1(x, y) = e_s^1 e^{\pm ip y} \sqrt{m_0} x \quad \text{if} \ x > 0,
\]

and only one bounded exponential mode order \( l \) in upper channels \( l > 1 \)

\[
f_s^l(x, y) = e_s^l e^{-ip \sqrt{\frac{m_0}{m_+} \frac{\pi^2(x^2 - 1)}{\delta^2} - p^2} x} \quad \text{if} \ x > 0,
\]

on the upper channels (spectral bands) \( l = 2, 3, \ldots \). The corresponding Scattering Ansatz in the wires \( \Omega_s \) is combined as

\[
\Psi_s(x) = \delta_s \Psi_{s1}^+ + f_{s1}^+ s_{s1}^1 + \sum_{l=2}^{\infty} s_{s1}^l f_{s1}^l
\]

(63)
with coefficients $S^1_{st}$ to be defined from the matching conditions with the corresponding solution of the above Schrödinger equation inside the quantum well $\Omega_0$. Choosing the outside positive normal on the boundary $\Gamma = \partial \Omega_0$, we can present the matching conditions with use of the standard Dirichlet-to-Neumann map (DN-map) of the quantum well $\Omega$. The above Ansatz (64) is already decomposed

$$\Psi_s = [\delta_{s1} f_1^- + S^1_{s1} f_1^+] + \sum_{l=2}^{\infty} S^1_{s1} f_s^l = \Psi^+_s + \Psi^-_s,$$

as a sum of vectors from $E_\pm$ respectively. Our aim is: to find the coefficients $S^1_{st}$ of the Ansatz which form the Scattering matrix. We may find them from the condition of the Scattering Ansatz inside the domain. Denoting by $\Psi^\gamma, \frac{\partial \Psi^\gamma}{\partial n}$, the boundary data of the above Scattering Ansatz on $\Gamma$, and assuming that the boundary values of the component $\Psi^\gamma$ of the scattered wave inside the quantum well coincide on bottom sections of wires with the boundary values of the Scattering Ansatz we may present these conditions with DN-map of the Schrödinger operator in $\Omega_0$:

$$\frac{m_0}{m^l} \frac{\partial \Psi_s^\gamma}{\partial n_\gamma} = \frac{\partial \Psi_s^\gamma}{\partial n_\gamma} = \Lambda^o_{\gamma} \Psi^\gamma_s.$$

(64)

Denote by $K^+, \bar{K}^+, K^-$ the operators in $E_+$ which compute the components of the normal derivatives of the exponential modes on the bottom sections of the wires $\Omega_s$ in the open and closed channel

$$K^+ = ip \sqrt{\frac{m^l}{m_0}} I, \quad K^- = -ip \sqrt{\frac{m^l}{m_0}} I$$

$$K^i_l = \sqrt{\frac{m^l}{m_0}} \sqrt{\frac{m^l}{m_0}} \frac{(l^2 - 1) \pi^2}{\delta^2} - p^2 I,$$

$l = 2, 3, \ldots, K^- = \text{diag} \{ K^i_l \}_{l=2}^{\infty},$

with positive square root, and by $P_\pm$ the orthogonal projections in $E$ onto the subspaces $E_\pm$. The matrices $K^+$ are $4 \times 4$ matrices proportional to the unit matrix, since potentials on the wires are equivalent. Then the above equation (64) may be presented as a matrix equation with respect to the components $\Psi^\pm_s$ of the above decomposition of $E = E_+ \oplus E_-$. Elements of the subspace $E_+$ belong to the Sobolev class $W^{1/2, 2}(\Gamma)$, hence the operators $P_+ \Lambda^o P_+, P_+ \Lambda^o P_-, P_- \Lambda^o P_+, P_- \Lambda^o P_-$ constructed via framing of the DN-map $\Lambda^o$ of the Schrödinger operator on the Quantum by projections onto entrance subspaces of open and closed channels exist as operators in proper classes. Denoting them by $\Lambda^o_{++}, \Lambda^o_{+-}, \Lambda^o_{-+}, \Lambda^o_{--}$ respectively, and by $S^1$ the $4 \times 4$ matrix with elements $S^1_{st}$ and set $(\Psi^+_s)_{s=1}^4(0) = \Psi^+, (\Psi^-_s)_{s=1}^4(0) = \sum_{l=2}^{\infty} S^1_l \Psi^+_s$.

**Theorem 10.2** The Scattering Matrix on the whole network $\Omega_0 \cup \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_4$ may be presented in terms of the Dirichlet-to-Neumann map $\Lambda^o$ of the quantum well $\Omega_0$ as

$$S(\lambda) = -\frac{\Lambda^o_{++} - \Lambda^o_{+-}}{K + \Lambda^o_{--} - \Lambda^o_{-+}} + \frac{1}{K - \Lambda^o_{--} + \Lambda^o_{-+}},$$

(65)

The Scattering Matrix may be presented as a function of the non-dimensional spectral parameter $\hat{\lambda} = R^2 \lambda$ which correspond to the scaled quantum well $\hat{\Omega}_0$ radius 1. The corresponding expression may be obtained as a Scattering Matrix of the scaled network via replacement of the DN-map $\Lambda^o (\lambda)$ of the quantum well $\Omega_0$ by the DN-map of the scaled domain $\Lambda^1(\hat{\lambda}) = R \Lambda^o (\lambda)$ and proper scaling of operators: $K^+ \to \hat{K}^+ = R K^+ $, $K^- \to \hat{K}^- = R K^-$, reducing the wires width $\delta$ to $\frac{1}{R}$:

$$\hat{S}(\hat{\lambda}) = -\frac{\Lambda^o_{++} - \Lambda^o_{+-}}{K + \Lambda^o_{--} - \Lambda^o_{-+}} + \frac{1}{K - \Lambda^o_{--} + \Lambda^o_{-+}},$$

(66)
Proof is obtained based on orthogonal decomposition of the whole space $L_2(\Gamma)$ into orthogonal sum of open and closed channels, followed by the straightforward calculation, see [34].

**Partial DN-map** The Scattering Matrix (66) contains a special combination of matrix elements of the DN-map $\hat{\Lambda}$ of the quantum well

$$\hat{\Lambda} = \hat{\Lambda}_{++} - \hat{\Lambda}_{+-} \frac{I}{K} + \hat{\Lambda}_{-+} - \hat{\Lambda}_{--}.$$  \hspace{1cm} (67)

This function has negative imaginary part in upper half-plane $\Im \lambda > 0$ and singularities at the vector-zeroes of the denominator $\left(K^{-} + \hat{\Lambda}_{-+}\right) e = 0$. The following statement, see [34], gives an interpretation of this function in terms of the intermediate operator $l'$:

**Theorem 10.3** The Intermediate operator $l'$ defined on the whole network $\Omega_0 \cup \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_4$ by the Schrödinger differential expression (47) and the boundary conditions (22) and (21) is self-adjoint. The continuous spectrum of the non-trivial component $l'$ of this operator on the orthogonal complement of the first channel consists of the branch $\lambda \geq \frac{m_0}{m_0} 3 \frac{\pi^2}{2}$ with the countable sequence of thresholds. With geometrical spectral variable $\lambda$ the eigenvalues of the operator $l'$ below the threshold $\frac{m_0}{m_0} 3 \frac{\pi^2}{2}$ coincide with the zeroes $\lambda^3$ of the denominator $\left(K^{-} + \hat{\Lambda}_{-+}\right)$. The DN-map of the operator $l'$ on the whole network with chopped-off first channel coincides with the operator-function (67).

This statement also can be verified via straightforward calculation, see [34] based on the fact that the intermediate operator is self-adjoint. Note that the DN-map of the intermediate operator is actually a finite matrix and it’s calculation requires only finite operations, eliminating infinite series: beginning from the Green function $\hat{G}'(x,y)$ of the self-adjoint intermediate operator $l'$ we consider the restriction of the corresponding Poisson map with the kernel $-\frac{\partial \hat{G}'}{\partial n}(x,y)$, $y \in \Gamma$ onto the 4-dimensional subspace $E_+^s$ of the entrance vectors $\bigcup_{s=1}^4 e_s$ of the open channels. Then anticipating the partial matching conditions $[20]$ in the open channel only we consider the projection of the normal derivative of the result on $\Gamma$ onto $E_+^s$ and obtain the kernel of the DN-map in form of $4 \times 4$ matrix from $E_+^s \times E_+^s$:

$$\hat{\Lambda}'(x',x,\lambda) = - P_+ \frac{\partial \hat{G}'}{\partial n_x} P_+$$ \hspace{1cm} (68)

Note that the vectors from the entrance subspace $E_+^s$ of the open channels, being continued by zero to the complement of the sum $\Gamma$ of bottom sections, belong to proper Sobolev classes on the whole boundary of the network so that the projection $P_+$ can be correctly calculated.

**Scattering matrix via partial DN-map** To calculate the Scattering matrix in terms of the partial DN-map of the Intermediate operator we should match the restriction of the Scattering Anzatz on the sum $\Gamma = \bigcup_{s=1}^4 \Gamma_s$ of bottom section of open channels only:

$$\Psi^+ = \delta_s \hat{f}_s + f^+_s \hat{S}_{s1}, \hspace{0.5cm} s = 1, 2, 3, 4,$$

$$\Psi = \left\{\Psi^+_s\right\}_{s=1}^4 = F_{in} e_i + F_{out} S e_i$$

with the Jost matrices $F_{in, out}$, to the solution $\Psi_0$ of the Intermediate homogeneous equation:

$$P_+ \Psi_0 = \Psi, \frac{1}{m_o} \frac{\partial \Psi_0}{\partial n_o} = \frac{1}{m_i} \frac{\partial \Psi_0}{\partial n_i}, \hspace{0.5cm} s = 1, 2, 3, 4.$$  \hspace{1cm} (69)

Substituting here the above expression (67) for the partial DN-map, and using the fact that all wires are equivalent, hence the Jost matrices are proportional to the unit matrix in open channels, we obtain an equation for the Scattering matrix:

$$\frac{1}{m_o} \hat{\Lambda} F_{in} - \frac{1}{m_i} F_{in} = - \left( \frac{1}{m_o} \hat{\Lambda} F_{out} - \frac{1}{m_i} F_{out} \right),$$

27
which has the solution:

\[ S = \frac{F_{in}}{F_{out}} \frac{\Lambda' - \frac{m_p E'}{m'} F_{in}}{\Lambda' - \frac{m_p E'}{m'} F_{out}} \]

where the denominator is preceding the numerator, and the fractions \( \frac{F_{in}}{F_{out}} \) are proportional to the unit matrix in \( E_\perp \). Substituting here the explicit expression for the Jost solutions in the open channel we obtain the expression (25) for the Scattering matrix in terms of DN-map of the intermediate operator.

Note that using of the partial DN-map of the intermediate operator automatically provides the matching conditions in closed channels.

10.3 Compensation of singularities

Singularities of the Scattering matrix sit near the eigenvalues of the Intermediate operator, which are shifted with respect to eigenvalues of the Schrödinger operator with Dirichlet boundary conditions on the boundary of the well. The shift, generically, is not large, but may be essential when searching for the working point. It may be estimated via standard analytical perturbation procedure.

**Theorem 10.4** The pole \( \lambda_0 \) of the DN-map \( \Lambda^0 \) of the quantum well, which is the singularity of the first addendum \( \Lambda'_{++} \) of (74), is compensated by the pole of the second addendum and disappears as a singularity of the whole function \( \Lambda' \), so that the whole expression (74) is, generically, regular at the point \( \lambda_0 \). A new pole appears as a zero of the denominator \( K^- \Lambda''_{--} \) and coincides with the eigenvalue of the intermediate operator. The corresponding residue is combined of root vectors which correspond to this new pole and disappear as a singularity of the whole function which has the solution:

\[ S = \frac{F_{in}}{F_{out}} \frac{\Lambda' - \frac{m_p E'}{m'} F_{in}}{\Lambda' - \frac{m_p E'}{m'} F_{out}} \]

and the corresponding non-dimensional wave-number \( \tilde{p} = Rp \) is

\[ \tilde{p} = Rp = \pi \frac{R}{\delta} \sqrt{\frac{3m_0}{2m^\perp}} \approx \frac{8.8 R}{\delta} \]

Practically it contains a “large” parameter compared with non-dimensional inverse spacing \( |\lambda_0 - \lambda_1|^{-1} = \frac{10}{2.3} \) already for \( R > \delta/2 \):

\[ \frac{10}{2.3} = 4.3 << 17.6. \]

For \( R = 10\delta \) the corresponding inequality is \( 4.3 << 88 \). For the normalized eigenvectors \( \hat{\phi}_s \) of the Dirichlet problem in the modified well \( \Omega_0 \) radius 1, with flattened pieces of boundary and properly transformed eigenfunctions, see suggestion above in 3.2, we introduce the unified notations:

\[ \phi_0 = \hat{\phi}_s \hat{\phi}_s = P_\pm \partial \hat{\phi}_s / \partial n, \]

and separate the resonance term in the DN-map framed by projections onto \( E_\pm \):

\[ P_+ \hat{\Lambda} P_+ = \frac{\phi_0^+}{\lambda - \lambda_0} + \sum_{s \neq 0} \frac{\phi_0^+}{\lambda - \lambda_s} := \frac{\hat{\phi}_0^+}{\lambda - \lambda_0} + \hat{K}_{++} \]

28
we obtain an explicit expression for the inverse operator \( K \). In particular, estimating the contribution \( \hat{L} \) with above assumption. Really, solving the equation

\[
P^{-1} = \frac{\hat{\phi}^+}{\hat{\phi}^-} + \sum_{s \neq 0} \frac{\hat{\phi}^+}{\lambda - \lambda_s} \hat{\phi}^- \equiv \frac{\hat{\phi}^+}{\lambda - \lambda_0} + \hat{K}^- \]

Then non-dimensional expression \( \| \) may be presented as

\[
R \lambda^r = \hat{\lambda}^r = \frac{\hat{\phi}^+}{\lambda - \lambda_0} + \hat{K}^- + \left[ \frac{\hat{\phi}^+}{\lambda - \lambda_0} + \hat{K}^- \right] \frac{I}{\hat{\phi}^+ / (\lambda - \lambda_0) + \hat{K}^- + \sqrt{m_{\|} / m_{\perp} R K^{-}} \hat{\phi}^- / (\lambda - \lambda_0) + \hat{K}^-}.
\] (71)

The operator \( R K^{-} = \hat{K}^- \) for selected value of energy is positive and may be estimated from below by the non-dimensional distance from the Fermi-level to the second threshold with (non-dimensional) coefficient \( \frac{\hat{\phi}}{\rho} \):

\[
\hat{K}^- \geq \sqrt{\frac{3 m_{\|}}{2 m_{\perp} R I}}.
\]

In particular, estimating the contribution \( \hat{K} \) from the non-resonance terms to DN-map as \( \| \hat{K} \| \leq \hat{\phi}^{-} / \rho(\lambda_0) \), we may conclude that

\[
\| \left[ \hat{\phi}^- / (\lambda - \lambda_0) + \hat{K}^- \right] \| \leq \sqrt{\frac{2 m_{\perp}}{3 m_{\|} \pi \rho(\lambda_0)}} \frac{\hat{\phi}^{-} / \rho(\lambda_0)}{\hat{\phi}}.
\] (72)

Assuming that \( m_{\perp} = 0.190 \), \( m_{\|} = 0.916 m_0 \), (for Si) \( \hat{\phi}^{-} / \rho(\lambda_0) = 2.3, \delta = 2 nm, R = 10 nm \), we obtain in the right side of (12) a “small” non-dimensional parameter \( \epsilon \approx 0.1 \) which may be used when developing a perturbation procedure. In particular we may calculate the inverse of \( \left[ \hat{\phi}^- / (\lambda - \lambda_0) + \hat{K}^- \right] \) estimating \( (\hat{K}^- + \hat{K}^-)^{-1} : k(\delta, R) := k \) as

\[
\| k \| \leq \frac{\delta}{R \pi \sqrt{3 m_{\perp}}} \quad \text{or} \quad \| k_{\delta, R} \| \leq 0.14 \frac{\delta}{R}
\]

with above assumption. Really, solving the equation

\[
\left[ \hat{\phi}^- / (\lambda - \lambda_0) + \hat{K}^- \right] u = f,
\]

we obtain an explicit expression for the inverse operator

\[
u = \left[ \hat{\phi}^- / (\lambda - \lambda_0) + \hat{K}^- \right]^{-1} f = k f - \frac{1}{D} k \hat{\phi}^- \left\langle \hat{\phi}^- , k f \right\rangle,
\]

where \( D = \hat{\lambda} - \lambda_0 + \left\langle \hat{\phi}^- , k \hat{\phi}^- \right\rangle \). Substituting that expression into (14), we notice that all terms containing \( (\hat{\lambda} - \lambda_0) \) in denominator are cancelled and we obtain:

\[
\hat{\lambda}_r = \frac{\hat{\phi}_r^-}{\hat{\phi}_r^-} \left\langle \hat{\phi}_r^- \right\rangle / \lambda - \lambda_0 = \frac{\hat{\phi}_r^+}{\hat{\phi}_r^-} \left\langle \hat{\phi}_r^+ \right\rangle / D,
\]

with the residue of the DN-map proportional to \( \hat{\phi}_r^+ \left\langle \hat{\phi}_r^+ \right\rangle \), as announced. The eigenvalues \( \hat{\lambda}_r \) of the operator \( \hat{\lambda}_r \) can be obtained from the equation \( D(\hat{\lambda}_r) = 0 \). The first order correction gives due to (10) \( |\hat{\lambda}_r - \lambda_0| \leq \frac{||\hat{\phi}^-||^2}{4} \approx 0.023 \ll 2.3 \), in agreement with the corresponding direct calculation \( \text{[37]} \).
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