Resonance Quantum Gate

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Abstract

Simplest models of two- and three-terminal Quantum Quantum Gates are suggested in form of a quantum ring with few one-dimensional quantum wires attached to it and several point-wise governing electrodes inside the ring which are charged by a single hole. In resonance case, when the Fermi level in the wires coincides with the resonance energy level on the ring the geometry of the device may be chosen such that the quantum current through the switch from up-leading wire to the outgoing wires may be controlled via re-directing of the hole from one governing electrode to another one. The working parameters of the gate are defined in dependence of the desired working temperature, the Fermi level and the effective mass of the electron in the wires.

1 Scattering problem and the switching effect

Modern quantum electronic devices may be manufactured as quantum networks of Aharonov-Bohm quantum rings and quantum wires formed on the surface of a semiconductor. Elements of these networks - rings and wires- may be obtained in self-assembled quantum wells inside Silicon wafer via controlled diffusion of borons with surface injection of vacancies, under proper temperature, see for instance [21], [22], [23]. The width of the rings and wires 20 Å is small comparing with De-Broghlie wavelength (80 - 150 Å) on the Fermi level, hence the network is quasi-one-dimensional. This permits to use the Schrödinger equation on the corresponding one-dimensional graph as a convenient model when exploring the quantum conductivity. The spectral theory of Schrödinger equation on the one-dimensional graph was developed in frames of the Theory of Operator Extensions in [11], [8], [7], [15], [16], [9]. Using of this approach in mathematical design of nano-electronic devices gives prediction of qualitative features of devices and even preliminary estimation of their working parameters. Interference of the wave functions served a base for design of the first patented quantum switch, see [10]. Basic problems of the mathematical design of quantum electronic devices were formulated in terms of quantum scattering in the beginning of nineties by [22]. Design of most of modern resonance quantum devices, beginning from classical Esaki diode up to the modern devices, see, for instance, [27], were based on the resonance of energy levels rather than on resonance properties of the corresponding wave functions. At the same time modern experimental technique already permits to observe resonance effects caused by details of the shape of the resonance wave functions, see [21], [22], [23]. In [17] the problem of resonance manipulation of quantum current through the quantum switch implemented as a quantum ring with few incoming/outgoing quantum wires was considered in frames of the relevant scattering problem. It was shown there, that the transmission from one (incoming) wire to another (outgoing) wire is defined not only by the position
of the resonance eigenvalue \(^2\) on the ring, but also by the \textit{shape of the corresponding resonance eigenfunction}. In frames of the EC-project "New technologies for narrow-gap semiconductors" (ESPRIT-28890 NTCONGS, 1998 - 1999) the problem on mathematical design of a four-terminal Quantum Switch for triadic logic was formulated by Professor G. Metakides and Doctor R.Compano from the Industrial Department of the European Comission. Results of the theoretical part of the project were published in papers \([17]\), \([18]\), \([19]\). In \([20]\), \([26]\) \([24]\) a new design of Resonance Quantum Switches (RQS) was suggested in form of a quantum domain or quantum ring with a few quantum wires (terminals) attached to it. The idea of the new design, as presented in \([20]\) and \([24]\) for the device designed in form of a quantum domain (quantum well), is based on the phenomenon observed first, see \([6]\), in the scattering problem for acoustic scattering on a resonator with a small opening: an additional term in the scattering amplitude caused by the opening appeared to be proportional to the value of the resonance eigenfunction at the opening (for the Neumann boundary condition on the walls of the resonator) or to the value of it’s normal derivative (for the Dirichlet boundary conditions), see \([25]\).

In \([24]\) the single act of computation - the switching of the current - is considered as a scattering process. In the corresponding mathematical scattering problem for the RQS on the graph formed as a ring of radius \(R\) and a few (straight) quantum wires weakly connected to it at the contact points \(a_s\) via tunneling of electrons of mass \(m\) across the potential barriers width \(l\), hight \(H\), the resonance eigenvalue \(E_2 = E_f\) on the ring is embedded into continuous spectrum of the Schrödinger operator on the whole graph. The width of the the part of the up-leading channel connecting the wire and the well, and hence the power of the potential barrier may be controlled by a special nano-electronic construction – the \textit{split-gate}. On the other hand the power of the potential barrier inside the split-gate may be manipulated by the classical electric field applied to the brush of boron’s dipoles sitting on the shores of the channel. This construction was suggested in experimental papers \([21]\), \([22]\), \([23]\), \([26]\). The hight of the barrier, and hence the power of it, is defined by the position of the lowest energy level in the cross-section of the channel of variable width.

If the potential barriers separating the wires from the ring are strong enough, then the connection between the wires and the ring may be reduced to the boundary condition with the small parameter

\[
\beta = \left( \cosh \frac{\sqrt{2mH}}{\hbar} l \right)^{-1}
\]

at the contact points \(a_s\). Here \(H\) is the hight of the barrier above the Fermi level and \(l\) is the width of it. For weak connection between the ring and the wires the transmission coefficient from one wire to another in the resonance case appears to be proportional to the product of the values of the normalized resonance eigenfunctions \(\varphi(a_s)\) at the contact points see \([17]\). The resonance condition is fulfilled if the re-normalized energy level \(E \to \lambda = k^2 = (E - V_2) \frac{\hbar^2 R^2}{2m}\) (proportional to the depth of the quantum wires \(E - V_2\) with respect to the resonance eigenvalue \(E\)) is close to the re-normalized Fermi level \(E_f \to \lambda_f = (E_f - V_2) \frac{\hbar^2 R^2}{2m}\). If the connection between the ring and the wires is weak, \(\beta \ll 1\), then the following approximate expression in scaled variables, see below Section 3, is true for the transmission coefficient from the wire attached to \(a_s\) to the wire attached to \(a_t\):

\[
S_{s,t}(\lambda) = \frac{2k|\beta|^2}{k|\beta|^2|\mathbf{\varphi}|^2 - i(\lambda_f - \lambda)\varphi(a_s)\varphi(a_t)} + O(\beta^2), \ s \neq t.
\]

where \(|\mathbf{\varphi}|^2\) is the length of the \textit{channel-vector} \((\varphi a_1, \varphi a_2, \ldots \varphi a_4)\) the second term is uniformly small when \(\beta \to 0\), but the first one exhibits a nonuniform behaviour in dependence on ratio \((\lambda_f - \lambda)/\beta^2\).
The last formula being applied formally to the case \( \lambda = \lambda_f \) shows, that the transmission coefficient is approximately equal to
\[
S_{s,t}(\lambda) = \frac{2}{|\vec{\varphi}|^2} |\varphi(a_s)\varphi(a_t)| + O(\beta^2).
\]

The transmission coefficient is not continuous with respect to the re-normalized energy \( \lambda \) uniformly in \( \beta \). The physically significant values of the transmission coefficient for non-zero temperature \( T \) may be obtained via averaging over intervals \( |E - E_f| < \kappa T \) for relatively small and relatively large temperature. In the first case we still have:
\[
|S_{ij}(T)|^2 \approx \frac{2|\varphi(a_s)\varphi(a_t)|^2}{|\vec{\varphi}|^4}
\]
but in the second case, we have :
\[
|S_{ij}(T)|^2 \approx \frac{4|\varphi(a_s)\varphi(a_t)|^2}{|\vec{\varphi}|^4} \frac{1}{1 + \frac{\kappa^2 T^2}{\lambda^2 |\vec{\varphi}|^4}}.
\]

Hence for small \( \beta \) and non-zero temperatures the averaged transmission coefficient is small, according to natural physical expectations.

Nevertheless the above formulae show that in certain range of temperatures the transmission is proportional to the product of values of the resonance eigenfunctions at the contact points. Similar observation takes place for switches based on the quantum well with Neumann boundary conditions, see [24] and analog of it with normal derivatives of the resonance eigenfunction remains true for the Dirichlet boundary conditions, see [25].

One may obviously construct the dyadic RQS basing on this observation. But even triadic (four-terminal) RQS may be constructed with minimal alteration of the geometrical construction. For instance, on a circular quantum well \( \Omega_0 \) : \( |\vec{x}| \leq R \) the magnitude of the constant electric field \( \mathcal{E}\vec{\nu} \), \( |\vec{\nu}| = 1 \), and the shift potential \( V_0 \), see [24], may be chosen such that the corresponding Schrödinger equation
\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + (\mathcal{E}e(\vec{x}, \vec{\nu}) + V_0) \psi = E\psi
\]
may have a resonance eigenfunction with an eigenvalue equal to the Fermi level \( E = E_f \) in the wires such that it has only one smooth line of zeroes which crosses the circle dividing it in ratio 1 : 2. Then, attaching the wires \( \Gamma \) to the domain at the points \( a_1, a_2, a_3, a_4 \) characterized by the central angles \( 0, \pm \pi/3, \pi \) we obtain the Resonance Quantum Switch manipulated by rotating \( \vec{\nu} \rightarrow \vec{\nu}' \) of the constant electric field \( \mathcal{E}\vec{\nu} \) in the plane parallel to the plane of the device. In particular, if for some direction \( \vec{\nu} \) the line of zeroes arrives to the boundary exactly at the contact points : \( a_2, a_3 \) (or \( a_3, a_4 \), or else \( a_4, a_2 \) ), then the corresponding wires \( \Gamma_2, \Gamma_3 \) (or respectively \( \Gamma_3, \Gamma_4 \), or else \( \Gamma_4, \Gamma_2 \)) are blocked. With two outgoing wires blocked, one up-leading wire \( \Gamma_1 \) and one outgoing wire (respectively \( \Gamma_4, \) or \( \Gamma_2, \) or \( \Gamma_3 \)) remain open. Hence the electron current may go across the well from the up-leading wire to the outgoing wire. The corresponding transmission and reflection coefficients may be calculated in course of solution of the corresponding scattering problem, [24].

For fixed contact points the working regime of the RQS is defined by the position of the working point \( R, \mathcal{E}, V_0 \) in the three-dimensional space of the parameters. This position is uniquely defined, see Section 4, by the desired working temperature \( T \) and by the Fermi level \( E_f \) in the up-leading quantum wires. Note, that the position of the working point can’t be defined experimentally just by naive scanning on one of parameters for other parameters fixed at random, since the probability of proper choice of the remaining parameters is zero (proportional to the zero-measure of a point on a \( 2 - d \) plane).
In the contrary to the Quantum Switch, the Quantum Gate we shall discuss is manipulated not by the classical electric field, but by an injection of a single quantum charged particle (a hole) into one of governing electrodes situated inside the ring. For the triadic (three-terminal) Resonance Quantum Gate the problem of choosing of position of the governing electrodes inside the ring is actually a sort of inverse problem for the corresponding quantum network. This problem may be formulated the following way:

Choose positions of the governing electrodes inside the ring and the height of them above the plane of the ring such that

1. The resonance eigenfunction on the ring has two zeroes which divide the ring in ratio $2 \div 1$.
   
   The position of the zeroes may be controlled by the charging of one of electrodes with a single hole such that the zeroes of the resonance eigenfunction block two of outgoing channels, leaving only one of outgoing channels open.

Solution of this inverse problem is non-unique. One of possible solutions is suggested in the next section 3 of our paper.

The plan of our paper is the following. In the second Section we suggest a solution of a problem of the geometrical design of a triadic Resonance Quantum Gate in a form of a circular quantum well with three point-wise electrodes inside of it. In the third section, following our previous results in [28], we define the small parameter in the boundary conditions. In the last Section 4 we calculate the the working parameters of the ring-based three-terminal Quantum Gate, manipulated by the single-hole charging of electrodes situated inside the ring.

We skip here discussion of two most important problems of the mathematical design of the Resonance Quantum Switches and Gates:

The calculation of the Voltage-Current characteristics and

The estimation of affordable precision of the geometrical details of it.

2 Resonance Quantum Gate

The Resonance Quantum Switch manipulated by the macroscopic electric field is actually a classical device for manipulating of quantum current. It can’t be used as a detail of a quantum network since the macroscopic electric field can't appear in the quantum network. In this section we consider a completely quantum device manipulated by a single electron or hole. Mathematical modeling of this device requires solution of a two-electron problem on a network, similar to one solved in the simplest case in [13]. In this note we consider a one-body version of the problem, assuming that a single hole is sitting inside the circular ring at the height $h$ over some point $b_s$ on the continuation of one of the radii corresponding to the contact point $a_s$ with outgoing wires at the distance $|b_s| = b$ from the center of the ring. We may have three electrodes inside the ring, and following three possible potentials which may be used for redirecting of the electron current to three possible outgoing wires. The Coulomb potential on the ring, produced by the single charge sitting on one of electrodes, is, counting the charge of electron,

$$-\frac{e^2}{\sqrt{R^2 + h^2 + b^2 - 2bR \cos(\theta - \theta_s)}}.$$ 

If the condition $\frac{2bR}{R^2 + h^2 + b^2} << 1$ is fulfilled, then using the Taylor expansion we may find the approximate expression for the potential energy of the Schrödinger equation on the ring in form:

$$V_s^C(x) \approx -\frac{e^2}{\sqrt{R^2 + h^2 + b^2}}.$$
Neglecting the small addend we obtain the renormalized harmonic potential in form

$$V_s(x) = -Q \cos(\theta - \theta_s) - A,$$

and thus we arrive again to the Mathieu equation with the potential $E e(\bar{x}, \bar{v})$ which will be analysed in the last section. After introducing the new variable $z = 1/2 (\theta - \theta_s)$ the coefficients of the Mathieu equation

$$y'' + (a - 2q \cos(2z))y = 0$$

are calculated as

$$a = \frac{8mR^2}{h^2} \left( E + \frac{e^2}{\sqrt{R^2 + h^2 + b^2}} \right),$$

$$q = -\frac{4me^2bR^3}{h^2(R^2 + h^2 + b^2)^{3/2}}.$$

Calculation of the working parameters will be accomplished in the last part of the section 3.

The above one-body approximation may be used if the life-time of the single hole on the electrode is greater than the life-time of the resonance, but still small enough to provide necessary speed of switching. If this condition is not fulfilled, then the corresponding two-body scattering problem should be analysed similarly to [13].

### 3 Boundary conditions at the contact points.

In this Section, following [28] we calculate the parameter $\beta$ in the boundary conditions for the RQG based on the quantum ring with few terminals. We assume that the potential barrier separating the ring from the quantum wire at the contact point may be controlled by the split-gate mentioned above, Section 1, see also [22], [23].

Consider a quantum gate constructed in form of a circular ring of quasi-one-dimensional quantum wire $\Gamma_0$ with a few straight radial up-leading wires $\Gamma_s = \Gamma_{s1} \cup \Gamma_{s2}$ attached to it orthogonally at the contact points $a_s$, $s = 1, 2, \ldots, 4$. The Schrödinger equation on the ring $\Gamma_0$ is defined by some smooth potential $q(x) + V_0$, and the Schrödinger equations on the wires $\Gamma_s = \Gamma_{s1} \cup \Gamma_{s2}$ have piecewise constant potentials

$$V_s(x) = \begin{cases} V_1, & \text{if } x \in \Gamma_1: -l < x < 0, \\ V_2, & \text{if } x \in \Gamma_2: 0 < x < \infty. \end{cases}$$

The point $x = -l$ on the wire $\Gamma_s$ coincides with the corresponding contact point $a_s$ on the ring $\Gamma_0$. The height $H = V_1 - E_f$ of the potential over the Fermi level on the initial part of the quantum wire (within the split-gate $x \in (-l, 0)$) is controlled by the electric field orthogonal to the wire, which may change the width of the the channel via turning the boron’s dipoles sitting on the shore of it [21], [22]. We assume, that the Fermi level in the wires lies between $V_1, V_2$: $H > 0 > V_2$, the boundary condition at the point of contact is chosen in Kirchhoff form\(^3\):

$$[u'_0'(a_s) + u_s'(a_s)] = 0,$$

\(^3\)In fact one may show that the boundary condition connecting the solutions of the differential equations on the wires and on the ring at the contact points depends on local geometry of the joining. We consider the Kirchhoff condition as a zero-order approximation for more realistic boundary conditions.
and the solutions \( u_s = \{u_{s1}, u_{s2}\} \) of the Schrödinger equations on \( \Gamma_s = \{\Gamma_{s1}, \Gamma_{s2}\} \) are smooth functions on the joint interval \((-l, 0) \cup (0, \infty) = \Gamma_1 \cup \Gamma_2\) for which the matching conditions are fulfilled

\[
u_{s1}(-0) = u_{s2}(0), \quad u'_{s1}(-0) = u'_{s2}(0).
\]

For “relatively low” temperature \( \kappa \Theta < \frac{\phi}{2} \), see below, section 4, one may assume that the dynamics of electrons is described as the restriction of the evolution defined by the non-stationary Schrödinger equation onto the spectral interval length \( \kappa T \) near the Fermi level (that is near the corresponding resonance eigenvalue on the ring). Practically we should calculate the scattering matrix on the graph for values of energy inside this interval. Following [28] we shall use the Ansatz for the component of the scattered wave on the ring in form of a linear combination of the Green functions of a perturbed problem which takes into account the presence of wires supplied with split-gates. We assume that the potential of the split-gate is strong enough \( \sqrt{2m(V_1 - E_f)} \bar{h} \geq r_l > 1 \) and \( e^{-\sqrt{2m(V_1 - E_f)} \bar{h} l} \ll 1 \). The presence of the wires with split-gates may be modeled by additional singular potential on the ring localized at the contact points. This potential was calculated in [28] from the Kirchhoff conditions for the solutions \( \psi, \psi_s \) of the Schrödinger equation on the ring and the Schrödinger equation on the wires at the contact points

\[
[\psi'](a_s) + \psi'|_{-l} = 0, \quad \psi|_{a_s} = \psi|_{-l}.
\]

If the potential barrier, defined by the split-gate in the initial part of the wire is strong enough, \( r_l > 1 \), then the solution of the Schrödinger equation with the constant potential \( V_1 \) on the initial interval \((-l, 0)\) of the wire may be approximated by an exponential:

\[
\psi_s = Ce^{-\sqrt{2m(V_1 - E_f)} \bar{h} (x+l)}.
\]

Eliminating the Cauchy data of the decreasing exponential solution on the wire we obtain from the above Kirchhoff condition the the jumping boundary condition for the wave-function on the ring at the contact points:

\[
[\psi'] - \sqrt{\frac{2m(V_1 - E_f)}{\bar{h}}} \psi|_{a_s} = 0.
\]

This boundary condition may be also presented in form of an additional singular potential:

\[
V(x) \longrightarrow V(x) + \sum_{s=1}^{4} \delta(x - a_s) \frac{\hbar \sqrt{2m(V_1 - E_f)}}{2m} := \tilde{V}(x).
\]

Constructing of the Green function of the “perturbed” Schrödinger operator

\[
\tilde{L} = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x) \psi + \sum_{s=0}^{4} \delta(x - a_s) \frac{\hbar \sqrt{2m(V_1 - E_f)}}{2m} \psi
\]

on the ring with the new potential \( \tilde{V} \) serves as a convenient step to construct the scattered waves on the whole graph.

Note that the Kirchhoff boundary condition imposed at the contact point \( a \), which has the coordinate \( x = -l \) on the corresponding wire may be transformed to the point \( x = 0 \) of the wire with use of the corresponding transfer-matrix for the Schrödinger equation on the wire \( \Gamma_s \). It is convenient to use the scaled variables on the ring \( x \rightarrow \frac{x}{\bar{r}} \) and on the wires \( x_s \rightarrow \xi = \frac{x_s}{\bar{r}} \). Denoting by
\[ \psi \] the symplectic variables of the component of the scattered wave at the contact point \( a_s/R \) on the scaled ring and by \( \tilde{\psi}_s, -\frac{\partial \tilde{\psi}}{\partial \xi} \), the symplectic variables of the component of the scattered wave on the scaled wire at the end of the split-gate \( \xi = 0 \), we obtain from the Kirchhoff condition the following boundary condition:

\[
\left( \frac{[d\tilde{\psi}_0]}{d\xi}(a_s/R) \right) = \left( \frac{Rr \tanh rl}{\cosh rl} \right) \left( \frac{1}{\tanh rl} \right) \left( \tilde{\psi}_0(a_s/R) \right) + \frac{1}{\cosh rl} \left( \frac{\partial \tilde{\psi}_0}{\partial \xi}(0) \right).
\]

(4)

Denote by \( \tilde{g}(\xi, \eta) \) the Green function of the scaled perturbed Schrödinger equation on the scaled ring. Then the jump of the derivative of it is equal to \(-1\) at all points on the unit circle, except contact points, where the jump is calculated as:

\[
[\tilde{g}']_{\xi=a_s/R} - rR\tilde{g}(a_s/R, a_s/R) = -1.
\]

We choose an Ansatz for the component \( \tilde{\psi}_0(\xi) \) of the scattered wave on the ring in form

\[
\tilde{\psi}_0(\xi) = \sum_{s=1}^{4} \tilde{g}(\xi, a_s/R)u_s^0 = \tilde{g}(\xi)u_0.
\]

Substituting now the corresponding component of the Ansatz \( \tilde{g}(a_s/R)u_0^0 := \{\tilde{g}u_0\}_s \) instead of \( \tilde{\psi}_0(a_s) \), and the \( s \)-component of the standard Ansatz \( e^{ik\xi} + S(k)e^{-ik\xi} \) \( \tilde{e} \) of the scattered wave for \( \tilde{\psi}_s \):

\[
\tilde{\psi}(0) = ([I + S]\tilde{e})_s := u_s(0), \quad \tilde{\psi}'(0) = ik([I - S]\tilde{e})_s := u'_s(0),
\]

into the above boundary condition we obtain the equation for the Scattering matrix:

\[
\left( \begin{array}{c}
\tilde{u}(0) - \frac{\tilde{u}_0}{Rr}d\tilde{u}'(0)
\end{array} \right) = \left( \begin{array}{cc}
Rr & -\frac{1}{\cosh rl} \\
\frac{1}{\cosh rl} & -\frac{1}{\cosh rl}
\end{array} \right) \left( \begin{array}{c}
\tilde{g}\tilde{u}_0 \\
-ik[I - S]\tilde{e}
\end{array} \right),
\]

(5)

where \( \tilde{g} \) is a matrix combined of values of the perturbed scaled Green function \( \tilde{g}(a_s/R, at_s/R) \) at the contact points. The scattering matrix may be found from these equations via eliminating of the variables \( u_0^0 \) on the ring.

According to the above assumption the ratio \( 1/\cosh rl := \beta \) may play the role of a small parameter in the boundary condition. Then the diagonal elements of the matrix in the right-hand side of the last equation have the second exponential order, meanwhile the anti-diagonal elements are of the first exponential order. Neglecting the elements of second order we obtain the simplified version of the boundary conditions

\[
\left( \begin{array}{c}
\tilde{u}(0) - \frac{\tilde{u}_0}{Rr}d\tilde{u}'(0)
\end{array} \right) = \left( \begin{array}{cc}
0 & \frac{1}{\cosh rl} \\
\frac{1}{\cosh rl} & 0
\end{array} \right) \left( \begin{array}{c}
\tilde{g}\tilde{u}_0 \\
-\frac{1}{\cosh rl}
\end{array} \right),
\]

(6)

which coincides with the phenomenological boundary condition we used in the section 1 for calculating of the scattering matrix.

Taking into account that \( \tilde{u}(0) = \frac{ik([I - S]\tilde{e}]}{\cosh rl} \) we may solve the equation \( \tilde{g} \) with respect to the \( S\tilde{e} \) for any 4-vector \( \tilde{e} \) and then obtain an expression for the scattering matrix in form

\[
S(k) = \frac{\tilde{g}(\lambda)}{\cosh^2 rl} + \frac{1}{Rr} - \frac{1}{k},
\]

(7)

Here \( \tilde{g}(\lambda) \) is a matrix combined of values at the contact points of the Green-function of the scaled perturbed equation on the ring: \( \{\tilde{g}(\lambda)\}_s = \tilde{g}(a_s/R, at_s/R, \lambda), \lambda = k^2 \). Now, similarly to analysis
the values of the resonance eigenfunction \( \phi \):

\[
\tilde{g} = \frac{|\tilde{\varphi}_2|^2 P_2}{\mu_2 - \lambda} + K.
\]

Here \( P_2 \) is the orthogonal projection in 4-dimensional euclidean space onto the vector \( \tilde{\varphi}_2 \) formed of the values of the resonance eigenfunction \( \varphi_2 \) at the contact points; the non-singular addend \( K \) may be estimated similarly to [17]. If the condition of domination of the non-singular term \( K \) by the group of the leading terms is fulfilled, in a small real neighborhood of the resonance eigenvalue \( \mu_2 \), then one may pertain the leading terms only when calculating an approximate expression for the scattering matrix in this neighborhood:

\[
S_{\text{approx}}(k) = \frac{|\tilde{\varphi}_2|^2 P_2 + \cosh^2 rl (\frac{1}{Rr} - \frac{i}{ik})}{|\tilde{\varphi}_2|^2 P_2 + \cosh^2 rl (\frac{1}{Rr} + \frac{1}{ik})}.
\] (8)

This gives actually a convenient two-poles approximation for the scattering matrix and estimation of life time of resonances- the speed of the decay of the resonance terms in solution of the non-stationary Schrödinger equation. It suffice to calculate zeroes of the leading term in the numerator assuming that \( \cosh rl \gg 1 \). Using the notation \( \alpha = \pm \sqrt{\mu_2} \), we obtain two zeroes in lower half-plane:

\[
k \approx \alpha + \frac{irR}{i\alpha - rR} \frac{|\tilde{\varphi}_2|^2}{2\cosh^2 rl}.
\] (9)

The two-poles approximation follows from it, and the imaginary parts of zeroes define the inverse life time \( \tilde{\gamma} \) of the resonances. The scaled time \( \tau \) corresponding to the scaled equation and the real time \( t \) are connected by the formula \( k^2\tau = (E - V_2)t \), or \( t = \frac{2mR^2}{\hbar^2} \tau \). The exponential decay of the resonance states of both scaled and the non-scaled equations is defined by the behaviour of he exponential factor \( e^{ik^2\tau} = e^{3Rk^2\tau} e^{-3k^2\tau} \). The decreasing exponential factor may be rewritten with respect to real time as \( e^{3k^2\frac{R^2}{mR^2} t} \). Hence the role of the real inverse life time is played by \( \Im k^2 \frac{R^2}{mR^2} \) and may be calculated approximately for \( \cosh rl \gg 1 \) as

\[
\frac{\alpha r^2 \hbar^2 |\tilde{\varphi}_2|^2}{2m(\alpha^2 + r^2 R^2) \cosh^2 rl}.
\] (10)

For intermediate values of \( \cosh^2 rl \gg \frac{1}{\sqrt{1 + \frac{R^2}{\mu_2}}} \) one may simplify the expressions in both terms of the previous formula for the scattering matrix neglecting \( e^{-2rl} \) compared with \( \sqrt{1 + \frac{r^2 R^2}{\mu_2}} \). Then we obtain another convenient approximate expression for the approximate scattering matrix near the resonance eigenvalue \( \mu_2 \):

\[
S_{\text{approx}}(k) = \frac{3ik - Rr}{3ik + Rr} \frac{2\cosh^2 rl \frac{Rr - ik}{Rr - 3ik} + Rr \tilde{g}}{2\cosh^2 rl \frac{Rr + ik}{Rr + 3ik} + Rr \tilde{g}}.
\]

We shall discuss now a version of RQG based on a circular quantum ring \( \Gamma_0 \) of radius \( R \) with three outgoing straight radial quantum wires \( \Gamma_s, s = 1, 2, 3 \) attached to it at the points \( \varphi = \pm \pi/3, \pi \) via tunneling across the potential barriers controlled by the split-gates. We assume, that the up-leading quantum wire is supplied with so high potential barrier that the jump of the derivative of the wave-function on the ring at this point may be neglected when calculating the eigenvalues and eigenfunctions of the perturbed operator \( \tilde{L} \). Still we pertain the jumps at the contact points.

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of the outgoing channels $\varphi = \pm \pi / 3, \pi$, characterized by the potential barriers width $l$ and height $H = V_1 - E_f$ over the Fermi level $E_f$ in the radial quantum wires $\Gamma_s$. In this section we assume that RQS is manipulated by the constant macroscopic electric field $E\hat{v}$ which generates the potential $E c R(\hat{v}, x) + V_0$ in the Schrödinger equation on the ring $\vec{x} = R\zeta, |\zeta| = 1$. It is equivalent to the leading term of the electrostatic potential generated by the single hole sitting on the selected electrode. We assume as before that the influence of the field on the quantum wires is eliminated by some additional construction, so that the potential on the wires produced by the above field is equal to zero. It means that the Schrödinger equation on the network combined of the up-leading wire, the ring $\Gamma_0$ and outgoing wires $\Gamma_1, \Gamma_2, \Gamma_3$ may be written as a system of Mathieu equation on the ring $\Gamma_0$

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dx^2} + (E e(\nu, x) + V_0) u = E u, \quad u = u_0,$$

and the Schrödinger equation with the step-wise potential

$$V_s(x) = \begin{cases} 
H + E_f, & \text{if } -l < x < 0, \\
E_f + V_s, & \text{if } 0 \leq x < \infty, V < 0
\end{cases}$$

on the outgoing wires $\Gamma_s$, $s = 1, 2, 3$ and on the incoming wire $\Gamma_4$. We assume also, that the incoming wire $\Gamma_4$ is attached to the quantum ring at some point $a$ which is different from the above points $a_s$. The connection of the outgoing wires with the quantum ring is characterized by the “small” parameter $\beta = (\cosh \sqrt{2m(V_1 - E_f)}/\hbar)^{-1} << 1$.

An important engineering problem is actually the proper choice of the electric field $E$ such that the corresponding differential operator on the ring has an eigenfunction with special distribution of zeroes: the zeroes of the eigenfunction corresponding to the second smallest eigenvalue should divide the ring in ratio $1:2$. We assume that the potential barrier at the contact point $a_4$ with the incoming wire is so high that we may neglect the jump of the derivative of the perturbed operator $\hat{L}$ eigenfunction at this point. Then the whole potential of $\hat{L}$ on the ring is combined of the smooth potential defined by the macroscopic field $E$ and an additional singular potential appearing from the Kirchhoff’s conditions of smooth matching of the solution $\psi$ at the contact points $a_s$, $s = 1, 2, 3$ on the ring with proper solutions of the equations on the wires when the energy is fixed on the Fermi level $E = E_f$:

$$[\psi'_0] - \frac{\sqrt{2m(V_1 - E_f)}}{\hbar} \psi |_{a_s} = 0,$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + E e(\vec{x}, \vec{v}) + \sum_{s=1}^N \delta(x - a_s) \frac{\hbar \sqrt{2m(V_1 - E_f)}}{2m} \psi + (V_0 - V_2) \psi = E \psi.$$

We select the field $E$, and hence the geometry of the device such that the resonance eigenfunction for $E = E_f$ would have, for certain direction of the unit vector $\vec{v}$, two zeroes on the ring sitting at the points $\varphi = \pm \pi / 3$. When using the standard form of the scaled Mathieu equation with properly re-normalized coefficients $q = \frac{4m \sqrt{E_f R^3}}{\hbar^2}$, $a = \frac{8m R^2 (E - V_0 + V_2) \hbar^2}{2 \pi}$

$$y'' + (a - 2q \cos(2z)) y = 0,$$

we should pass from the angular (scaled) variable $\xi = x/R$ to the new variable $z = \frac{x}{2 R}$ which is changing on the interval $-\pi/2, \pi/2$. We have found that if the vector $\vec{v}$ is directed toward
z = 0, and the solution \( \psi \), we are looking for, is an even (cosine-type) solution of the Mathieu equation on the scaled ring \(-\pi/2 < z < \pi/2\) with a positive value at the point \( z = 0 \), and zeroes at \( z = \pm\pi/6 \), then it is smooth at the contact points with \( z = \pm\pi/6 \) and has a jump of the derivative 
\[ \tilde{\psi}'(\pi) = \frac{R\sqrt{2m(V_1 - E_f)}}{h} \bar{\nu} \tilde{\psi}(z) \]

at the point \( z = \pm\pi/6 \). Hence, \( y = \tilde{\psi}(z) \) satisfies the Mathieu equation on the interval \((0, \pi/2)\) and the boundary conditions
\[ dy/dz(\pi/2) + \frac{R\sqrt{2m(V_1 - E_f)}}{h} \tilde{\psi}(\pi/2) = 0. \]

The dimensionless Mathieu equation in standard form \([11]\) with properly scaled variable \( z \), \(-\pi/2 < z < \pi/2\), was analyzed with Mathematica in dependence of the re-normalized electric field and the parameter \( \gamma = \frac{R\sqrt{2m(V_1 - E_f)}}{h} \) in the boundary condition \( \frac{d\tilde{\psi}}{d\xi} - \gamma \tilde{\psi} = 0 \) at the contact points. It was found that for the following values of the parameters \( q, \gamma \) the resonance eigenfunction with two zeroes at \( z = \pm\pi/6 \) exists, for instance:
\[ \gamma = 10, \quad q = -1.98, \quad a = 5.24. \]

For the parameter \( q \) selected as shown above, there exist an eigenfunction \( u \) of the Mathieu equation perturbed by the \( \delta \)-potentials attached to the points \( a_s \) with weight \( \gamma \) such that the zeroes of \( u \) divide the unit circle in ratio \( 1 \div 2 \). These eigenfunctions may play a role of the resonance eigenfunctions for the corresponding triadic Resonance Quantum Gate. Being normalized by the condition \( \varphi(0) = 1 \) this function has square \( L_2 \)-norm 3.5234. The spacing between the resonance eigenvalue \( \mu_2 = \frac{4}{9} \) = 1.30 on the unit ring and the nearest eigenvalue \( \mu' = \frac{a^2}{4} = 1.49 \) (from the odd series of the eigenfunctions) is estimated as 0.19. Now the working temperature of the switch may be estimated as in the next Section 4: \( \kappa T \leq \frac{0.10 h^2}{4mR^2} \). For quantum rings with radius 10 nm the switching time estimated from the life time of the corresponding resonance may be circa \( 10^{-17} \) sec.

### 4 High-temperature triadic RQG

Consider a RQG constructed in form of a quantum domain - a circular quantum well - with four terminals - quantum wires - attached to it at the contact points \( a_1, a_2, a_3, a_4 \), selected as suggested above. To choose the working point of the switch in dependence of desired temperature we consider first the dimensionless Schrödinger equation
\[ -\Delta u + \epsilon(\tilde{\xi}, \tilde{\nu}) u = \lambda u \]

in the unit disc \( |\tilde{\xi}| < 1 \) with Neumann or Dirichlet boundary conditions at the boundary. The dimensionless Schrödinger equation may be obtained from the original equation by scaling \( \tilde{x} = RX \):
\[ -\Delta_{\tilde{\xi}} u + \frac{2m\epsilon R^3}{\hbar^2} \langle \tilde{\xi}, \tilde{\nu} \rangle u = \frac{2mR^2(E - V_0)}{\hbar^2} u. \]

Here \( \epsilon \) is the magnitude of the selected electric field and the unit vector \( \tilde{\nu} \) defines it’s direction, \( e \) is the absolute value of the electric charge of the electron and \( R \) is the radius of the circular well. Selecting \( \epsilon = \frac{2m\epsilon R^3}{\hbar^2} = 3.558 \) for Neumann boundary conditions one may see, \([24]\), that the
eigenfunction corresponding to the second lowest eigenvalue $\mu_2 = 3.79$ of the dimensionless equation (13) has only one smooth zero line in the unit disc which crosses the unit circle at the points situated on the ends of radii forming the angles $\pm \frac{\pi}{3}$ with the electric field $\vec{e}$. The minimal distance $\delta_0$ of $\mu_2$ to the nearest eigenvalues (the spacing of eigenvalues at $\mu_2$), depending on boundary condition on the border of the well, may be between 2 and 10. For Dirichlet or Neumann boundary conditions the eigenfunctions of the spectral problem for the above Schrödinger equation (13) are even or odd with respect to reflection in the normal plane containing the electric field $\vec{e}$. In particular for the Neumann boundary conditions the nearest eigenvalues corresponding to even eigenfunctions are equal $\mu_1 = -0.79$ and $\mu_3 = 9.39$, that it the spacing between $\mu_2$ and other eigenvalues of the even series may be estimated as $\delta_0 := \min\{|\mu_2 - \mu_1|, |\mu_2 - \mu_3|\} \approx 4$. Generally for the circular domain the spacing between the second lowest eigenvalue $\mu_2$ and other eigenvalues (of both even and odd series) may be estimated from below as $\delta_0 \geq 2$. The working regime of the switch will be stable if the bound states corresponding to the neighboring eigenvalues will not be excited at the temperature $T$:

$$\kappa T \frac{2mR^2}{\hbar^2} \leq \frac{\delta_0}{2}. \quad (15)$$

This condition may be formulated in terms of the scaled temperature $\Theta = \frac{2mR^2T}{\hbar^2}$ as

$$\kappa \Theta < \frac{\delta_0}{2}. \quad (16)$$

The temperature which fulfils the above condition we call low temperature for the given device. If the radius $R$ of the corresponding quantum well is small enough, then it may work at the (absolutely) high temperature, which correspond to the low scaled temperature. It may take place if the radius of the well is sufficiently small. 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 [27].

We assume that the effective depth $V_f$ of the bottom value $V_2$ of the potential on the wires from the Fermi-level $E_f$ in the wires is positive $V_f = E_f - V_2 > 0$, and the De-Broghlie wavelength on Fermi level is defined as

$$\Lambda_f = \frac{\hbar}{\sqrt{2mV_f}}.$$

Then we obtain the estimate of the radius $R$ of the domain from (13) as:

$$\frac{R}{\Lambda_f} \leq \sqrt{\frac{V_f}{\kappa T}} \sqrt{\frac{\delta_0}{8\pi^2}}. \quad (17)$$

For fixed radius $R$, the shift potential $V_0$ may be defined from the condition

$$\frac{2mR^2[E_f-V_0]}{\hbar^2} = \mu_2.$$

For instance, if we choose the radius $R$ of the domain as $R^2 = \frac{\delta_0 h^2}{4m\kappa T}$, we obtain:

$$V_0 = E_f - \frac{\hbar^2 \mu_2}{2mR^2} = E_f - 2\kappa T \frac{\mu_2}{\delta_0}.$$

Finally, the electric field $\mathcal{E}$ may be found from the condition

$$\epsilon = 3.8 = c\mathcal{E} \frac{2mR^3}{\hbar^2},$$

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where \( e \) is the absolute value of the electron charge. Hence for the value of \( R \) selected above we have:

\[
e E R = e \frac{\hbar^2}{2mR^2} = \frac{2e\kappa T}{\delta_0}.
\]

Hence the switch may work even at room temperature if the radius \( R \) of the quantum well is small enough and the geometrical details are exact.

Similar calculations may be done for the circular quantum well with Dirichlet boundary conditions. It appeared that for the dimensionless equation with the potential factor \( \epsilon = 18.86 \) the eigenfunction with a single zero-line dividing the unit circle into ratio 1 : 2 corresponds to the second smallest eigenvalue \( \mu_2 = 14.62 \). The lowest eigenvalue which corresponds to the even eigenfunction is \( \mu_1 = 2.09 \) and the spacing between \( \mu_2 \) and other eigenvalues of both even and odd series is estimated as before, \( \delta_0 \geq 2 \). This gives proper base for calculation of the radius of the quantum well, the intensity of the electric field and the shift potential subject to given temperature and the Fermi level.

References

[1] P. Lax, R. Phillips. *Scattering theory* Academic press, New York, 1967.

[2] I.S. Gohberg and E.I. Sigal. *Operator extension of the theorem about logarithmis residue and Rouche theorem*. Mat. sbornik. 84, 607 (1971).

[3] A. Baz’, J. Zeldovich, A. Perelomov. *Scattering, reactions and decay in non-relativistic quantum mechanics*. Nauka, 1971. 544 p., in Russian.

[4] M. Reed and B. Simon. *Methods of modern mathematical physics*. Academic press, New York, London, 1972.

[5] O. Madelung. *Introduction to solid-state theory*. Translated from German by B. C. Taylor. Springer Series in Solid-State Sciences, 2. Springer-Verlag, Berlin, New York, 1978. 486 p.

[6] M. Faddeev, B. Pavlov. *Scattering by resonator with the small opening*. Proc. LOMI, v126 (1983). (English Translation J. of Sov. Math. v27 (1984) pp 2527-2533)

[7] B. Pavlov. *The theory of extensions and explicitly solvable models*. Uspekhi Mat. Nauk, 42 (1987) pp 99–131.

[8] S. Albeverio, F. Gesztesy, R. Hoegh-Krohn, H. Holden, *Solvable models in quantum mechanics*. Springer-Verlag, New York, 1988.

[9] S. Albeverio, P. Kurasov. *Singular Perturbations of Differential Operators* London Math. Society Lecture notes Series 271. Cambridge University Press (2000) 429 pp

[10] P. Exner, P. Sheba. *A new type of quantum interference transistor*. Phys. Lett. A 129:8,9 pp 477-480.

[11] N. Gerasimenko, B. Pavlov. *Scattering problem on compact graphs*. Theor. and Math. Phys. 74 (1988) p 230.

[12] V. Adamjan. *Scattering matrices for microschemes*. Operator Theory: Adv. and Appl. 59 (1992) pp 1-10.
[13] Yu.B. Melnikov and B.S. Pavlov. *Two-body scattering on a graph and application to simple nano-electronic devices*. J. Math. Phys. **36**, 6, (1995) pp 2813-2825.

[14] R. Mennicken, A. Shkalikov. *Spectral decomposition of symmetric operator matrices*. Math. Nachrichten, **179** (1996) pp 259-273.

[15] S.P. Novikov. *Schrödinger operators on graphs and symplectic geometry*, in: The Arnol’dfest (Proceedings of the Fields Institute Conference in Honour of the 60th Birthday of Vladimir I. Arnol’d), eds. E. Bierstone, B. Khesin, A. Khovanski and J. Marsden, Communications of Fields Institute, AMS, 1999.

[16] V. Kostrykin and R. Schrader. *Kirchhoff’s rule for quantum wires*. J. Phys. A: Math. Gen. v32 (1999) pp 595-630.

[17] V. Bogevolnov, A. Mikhailova, B. Pavlov, A. Yafyasov. *About Scattering on the ring*, in: Operator Theory: Advances and Application, **124** (IWOTA-98: I.Gohberg’s Volume), Birkhauser Verlag, Basel, 2001.

[18] B.S. Pavlov, I.Yu. Popov, V.A. Geyler, O. Pershenko. *Possible construction of quantum multiplexer*. Europhys. Letters. **52** (2000).

[19] B.S. Pavlov, I.Yu. Popov, O.S. Pershenko. *Branching waveguides as possible element of quantum computer*. Priborostroenie. **43** (1-2) (2000) pp 31-34.

[20] Provisional Patent: *A System and Method for Resonance manipulation of Quantum Currents Through Splitting*, Auckland University Limited, 504590, 17 May 2000, New Zealand.

[21] N.T. Bagraev, V.K. Ivanov, L.E. Kljachkin, A.M. Malyarenko, I.A. Shelych. *Ballistic Conductance of a Quantum Wire at finite Temperatures*. Physics and techniques of semiconductors, v34 (2000) p 6.

[22] N.T. Bagraev, V.K. Ivanov, L.E. Kljachkin, A.M. Maljarenko, S.A. Rykov, I.A. Shelyh *Interferention of charge carriers in one-dimensional semiconductor rings*. Physics and techniques of semiconductors, v34 (2000) p 7.

[23] N.T. Bagraev, A.D. Bouravleuv, A.M. Malyarenko, S.A. Rykov. *Room temperature single-hole memory unit*. Journ. of low-dim. Structures. v9/10 (2000) pp 51-60.

[24] A. Mikhailova, B. Pavlov. *Quantum domain as a triadic relay*, in: Unconventional Models of Computations UMC’2K, (Proceedings of the UMC’2K Conference Brussels, Dec 2000) eds.I. Antoniou, C. Calude, M.J. Dinneen, Springer Verlag Series for Discrete Mathematics and Theoretical Computer Science (2001), pp 167-186.

[25] A. Mikhailova, B. Pavlov. *Resonance Quantum Switch*. Accepted for publication in : Proceedings of Sonja Kovalevskaja Conference, Stockholm, June 2000, Operator Theory: Advances and Applications, Ed. Birkhauser, Basel.

[26] B. Pavlov. *Mathematical design and prospects of an experimental implementation of a triadic quantum switch (Abstract)*. 7th MELARI/NID Workshop, Bellaterra, Barcelona, February 7-9 (2001), pp 40-42.

[27] European Comission IST programme: Future and emerging Technologies. *Technology Roadmap for Nanoelectronics*, R. Compano (ed.), Second edition, Nov. 2000. Luxemburg: Office for Official Publications of the European Communities. 105 p.
[28] N.Bagraev, A.Mikhailova, B.Pavlov, L.Prokhorov Resonance Quantum Switch and Quantum Gate Manuscript, 21p.