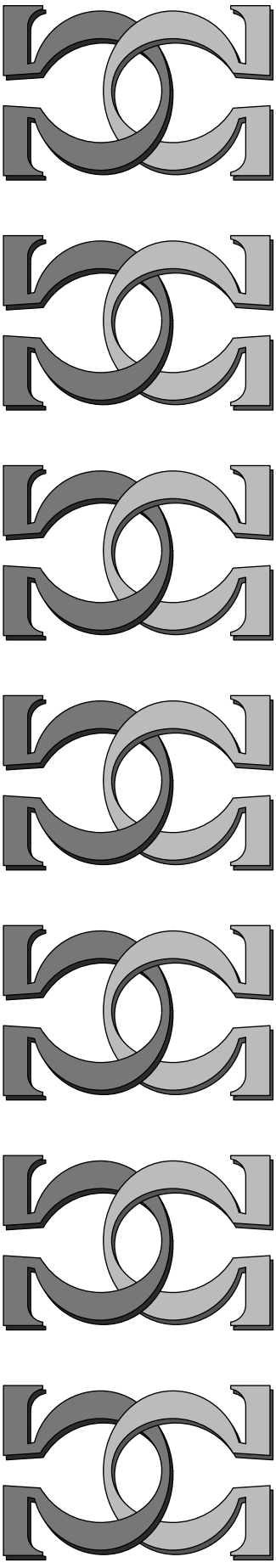

CDMTCS Research Report Series

Quantum Electronic Devices Based on Metal-Dielectric Transition in Low-Dimensional Quantum Structures

I. Antoniou, B. Pavlov, A. Yafyasov
Solvay Institute, Brussels, Belgium
University of Auckland, New Zealand
Institute for Physics, St. Petersburg University, Russia

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I. Antoniou
Solvay Institute, Brussels, Belgium
B. Pavlov,*__A. Yafyasov__
Institute for Physics, St. Petersburg University, Russia

1. Introduction. Recently P. Shor [1] discovered an efficient quantum "polynomial-time algorithm" (length $(\lg_2 N)^k$ for some finite k) for factoring large numbers N in the form of a product of prime factors. This event makes the implementation of more efficient quantum gates (see [2]) an actual problem of quantum engineering.

The quality of the implementation of the gates is characterized by the energy $E = \frac{1}{T_0}$ of interaction between pair of qubits and the damping rate $\Gamma = \frac{1}{\tau}$ for the coherence of any one qubit. The ratio of the single qubit coherence decay time τ ("coherence time") and the time T_0, required to perform the coherent change of state of qbits due to the interaction ("switching time") should be large for reversible coherent computations:

$$\frac{\tau}{T_0} >> 1.$$

The quantum coherence has been observed for tunnel-coupled systems of several quantum dots. The dominant mechanism destroying coherence at low temperatures is the electron-electron scattering, which is sensitive to the geometry of devices [3,4,5]. The above ratio for a single quantum dot is approximately 10^3 at Helium temperatures and could be improved if smaller quantum dots could be constructed.

The superconducting quantum interference devices, constructed as a system of superconducting rings with Josephson contacts between them are dual to the quantum dots, trapping magnetic flux instead of electrons, however the loss of coherence in those devices is not properly understood jet (see [6]).

Cirac and Zoller [7] proposed recently a laser-cooled array of Ions in the linear Pauly trap as a device for quantum computations. The coherence time for this device could be several seconds or even longer, and the switching time is defined by the optical transitions frequency.Thus the characteristic ratio of "coherence time" to "switching time" should be large at Helium temperatures. For modern discussion of other optical gates see [8].

It was shown (see for instance [9]), that only two types of operations -"gates"- are necessary to perform any quantum computation: the single bit "Rotate Operator" and two-bits "Controlled-Not Operator". In this paper we discuss the implementation of quantum gates "Controlled-Not" in the form of a quasi-molecular chain of atoms or clusters, controlled by some sort of optical excitation. Our analysis shows, that for proper choice of materials the working temperatures of the proposed device might be essentially higher, than the working temperatures of devices mentioned above.

The role of one of qubits in our device is played by the inner atomic electrons which are transferred simultaneously by optical excitation in all atoms of the chain from the ground state into the excited state, but still remain inside atoms; another qubit is represented by the asymptotic states (scattering states) of the conductivity electrons in quantum wires attached to the chain. In dependence of the occupation of inner orbitals the transmission coefficient might be (close to) zero or, to the transmission coefficient through semiinfinite periodic lattice. These cases correspond to the case of zero conductance of the device or, respectively, to the good conductance in accordance with Landauer formula [10,11].

*Actual address: Department of Mathematics, the University of Auckland, New Zealand.

The corresponding ratio is formed by the life-time of the excited state and the inverse optical frequency, and could vary in a wide range in dependence on the choice of materials.

Strictly speaking the scattering states of conductivity electrons are not representing qubits in proper sense, since the transmission coefficient through the chain could not be precisely 0 or modulo 1. Nevertheless we can show, that the proper choice of the materials and the parameters of the device makes them reasonable close to 0 or to the transmission coefficient T_∞ for semiinfinite lattice in dependence of the occupation of atomic orbitals. Due to the unitarity of the complete scattering matrix, the difference $1-|T_\infty|^2$ is equal, to the square modulo of the reflection coefficient from the infinite halflattice. Formally It plays the role of the relative measure of necessary "garbage" which should be stored and used when performing invertible computations. But in our case the reflection coefficient is an analytic function of energy, hence it can be restored from the orthogonality condition, in unique way, up to some unimodular Blashke-factor, which is trivial, if the bound states with negative energies are absent. Thus the nonzero transmission coefficient contains the complete information of the incoming signal, and *nothing* is lost in form of reflected wave, hence the computation act is reversible, though some part of the signal disappears forever.

The *irreversible* loss of information appeares when measuring the result of scattering by some classical device or even by some quantum device on a stochastic background. Then the part of information contained in the transmitted signal is destroyed and the computation *becomes irreversible*. More detailed discussion of comparison of quantum computations and classical computations on stochastic (Markov) background is contained in the last section 4.

We are discussing here one-electron approximation, assuming, that life-time of the inner cluster electrons is large enough, hence the occupation of cluster orbitals is changing by resonance laser shining only. But our model can be used beyond these limits as well, if we consider the corresponding two-electrons problem, as in [12]. It will be done elsewhere.

2. One-electron scattering by single quantum dot: Soluble model and physical reality. In this section we describe a soluble model of the simplest quantum "Controlled-not" quantum gate represented in the form a quasi-molecular cluster attached to some quantum wire by tunnel contacts. This model can be applied for theoretical analysis of constructions of nanoelectronic devices of narrow-band semiconductors.

We represent the one-electron Hamiltonian of quantum dot attached to the quantum wire as a result of perturbation of the orthogonal sum of "internal" and "external" Hamiltonians. The "internal" Hamiltonian of the electron in a cluster is determined by the occupation of the molecular orbitals

$$A_g \sim \alpha_e < \alpha_1 < \alpha_2 < \ldots; \quad A_g\phi_s^g = \alpha_s\phi_s^g$$

$$A_e \sim \alpha_g < \alpha_1 < \alpha_2 < \ldots; \quad A_e\phi_s^e = \alpha_s\phi_s^e.$$

Before the interaction is switched on, we represent the internal Hamiltonian by proper finite-dimensional operators (diagonal matrices) in each ground and excited states. The "external" Hamiltonian - the free Hamiltonian of an electron in a wire ("external channel") - is defined by the Schrödinger-type differential expression:

$$lU = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2U_0}{\mathrm{d}^2x},$$

where the effective electron mass m is determined both by the wire structure and the Fermi level λ_F energy near the conductivity band edge.

The quasi-molecular cluster attached to the wire could be represented of course by the equivalent potential well, separated from the outside of the wire by the potential barriers, simulating the Coulomb blockade, see [5]. But the analysis of solutions of the corresponding Schrödinger equation is generally possible either in the quasi-classical limit, which is rather far from realistic physical conditions, or for properly choosen soluble models. This is a reason why we use here a soluble model based on Operators Extensions Theory.

We use it here in form of so called *zero-range potentials with the inner structure*, proposed as an universal model for certain class of Schrödinger-type spectral problems in [13]. These models supply us with a wide range of spectrally interesting Hamiltonians and give us a realistic physical picture the spectrum and dynamics of perturbed systems, when the perturbations satisfy the following condition:

the de Broghlie wave-length in the nonperturbed system is greater, than typical dimensions δ of the perturbation considered

$$\delta << \lambda \approx \frac{2\pi\hbar}{\sqrt{2mkT}},$$

where m is the effective mass of electrons at the Fermi level.

In a certain sense this condition is similar to the condition of the slow phase change, formulated for mesoscopic processes by Altshuler (see [3]).

Our analysis shows, that the condition above holds for constructions of *narrow-gap and zero-gap semiconductors* , since for narrow-gap semiconductors the de Broglie wave-length, being inversely proportional to $\sqrt{m}$ which is essentially smaller, than the conventional mass of electron.

For the semiconductors presented in the following Table, the electron wavelength is some hundreds of Angstroms at the room temperatures and thousands of ones at the liquid nitrogen temperature. Creating relatively "small" clusters, which fulfill the above condition and can be considered as perturbations for quantum wires of these materials, is already possible using modern technical and technological tools: electronic lithography, ionic implantation, and selected chemical etching [14].

This allows our device to work at essentially higher temperatures as known world samples of quantum gates. Our calculations (see Section 3,[15]) are illustrated by the following Table.

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

Thus the properties of the mentioned semiconductive materials allow to realize the low-dimensional quantum system for temperatures *higher than the nitrogen boiling temperature*. The characteristic dimensions of such structures are available for the theoretical analysis of the construction of devices using the developed zero-range potential techniques and their fabrication by modern technology methods.

At the actual moment the basic problem requiring the experimental solution remains the problem of the influence of charge heterogeneities near the low-dimensional system. The possibility to achieve low densities of the charge heterogeneity was shown in our experiments for the Ge surface at the room temperature [18].

The proposed model can give us realistic spectral properties of objects under consideration, but of course *not the local differential properties of the solutions* of the corresponding Schrödinger equation, hence it is essentially "spectral modelling". On the other hand, our models help producing a lot of explicit formulas for spectral characteristics such as scattering matrices and resonances, both in asymptotically homogeneous and periodic cases.

According to the general scheme of the zero-range potentials with the internal structure, developed in [13], the connection of the model cluster determined by matrix A and the wire is described by the

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

boundary conditions, which connect the value of the external component of the wave function and its derivative jump

$$\left[\frac{\mathrm{d}U_0}{\mathrm{d}x}\right](0) = \frac{\mathrm{d}U_0}{\mathrm{d}x}(+0) - \frac{\mathrm{d}U_0}{\mathrm{d}x}(-0)$$

at the point 0 of connection of both channels (the cluster and the wire):

$$\left\{-U_0(0), \left[\frac{\mathrm{d}U_0}{\mathrm{d}x}\right](0)\right\}$$

to the *boundary values* $\xi_\pm$ of the internal component U_1 determined by the choice of the corresponding *deficiency vector* h in the *internal* (cluster) "channel":

$$U_1 = U_{10} + \frac{A}{A-iI}\xi_+ \cdot h + \frac{1}{A-iI}\xi_- \cdot h$$

$$(A-iI)U_{10} \perp h.$$

This boundary condition is given by some Hermitian matrix $\{\gamma_{ik}\}$, which is a parameter of the model as well:

$$\begin{pmatrix} -U_0(0) \\ \xi_- \end{pmatrix} = \begin{pmatrix} \gamma_{00} & \gamma_{01} \\ \gamma_{10} & \gamma_{11} \end{pmatrix} \begin{pmatrix} \left[\frac{\mathrm{d}U_0}{\mathrm{d}x}\right](0) \\ \xi_+ \end{pmatrix}.$$

The above boundary condition describes the electron's transition from the internal (cluster) channel to the external one $L_2(R)$ (the wire) and backwards. The operator l_A which is defined on the linear set of elements (U_0, U_1), which satisfy the above boundary condition

$$l_A \begin{pmatrix} U_0 \\ U_1 \end{pmatrix} = \begin{pmatrix} -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2U_0}{\mathrm{d}x^2} \\ AU_{10} - \frac{1}{A-iI}\xi_+ h + \frac{A}{A-iI}\xi_- h \end{pmatrix}$$

proves to be self-adjoint. It will serve as a Hamiltonian of a single electron in a wire with a cluster attached to it. This Hamiltonian can be used to describe the electron dynamics defined by the solutions of the corresponding nonstationary Schrödinger equation:

$$\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} U_0 \\ U_1 \end{pmatrix} = l_A \begin{pmatrix} U_0 \\ U_1 \end{pmatrix}.$$

The constructed model is obviously soluble: the eigenfunctions of the Hamiltonian can be given in an explicit form

$$\Psi_\lambda = \begin{pmatrix} \Psi^0_\lambda \\ \Psi^1_\lambda \end{pmatrix}.$$

In particular, for the scattered waves we have:

$$\Psi^0_\lambda = \begin{cases} \mathrm{e}^{ikx} + R\mathrm{e}^{-ikx}, x > 0, \\ T\mathrm{e}^{ikx}, x < 0;\ \lambda = k^2 \end{cases}$$

$$R = T - 1,$$

$$T(\lambda) = \frac{\frac{ik\hbar^2}{m}[\gamma_{00} - |\gamma_{01}|^2(\gamma_{11} - Q(\lambda))^{-1}]}{\frac{ik\hbar^2}{m}[\gamma_{00} - |\gamma_{01}|^2(\gamma_{11} - Q(\lambda))^{-1}] - 1},$$

$$\Psi^1_\lambda = \frac{A+iI}{A-\lambda I}h(Q(\lambda) - \gamma_{11})^{-1}\frac{\gamma_{10}}{m}\hbar^2(1-T).$$

Here $Q(\lambda) \equiv \langle \frac{1+\lambda A}{A-\lambda I}h, h\rangle$ is the rational function which has a positive imaginary part in the upper half-plane (and the negative one in the lower one). If the parameters of the model are connected by the condition

$$\gamma_{11} + \langle Ah, h\rangle = 0,$$

then the transmission coefficient T has the physically correct high energy asymptotic which is typical for the Schrödinger equation with smooth potentials:

$$T(k) = 1 + o(1/k).$$

The conductivity of the wire with the model cluster attached to it is given by the Landauer formula [10, 11]:

$$\sigma(\lambda) = \frac{e^2}{\hbar}\frac{|T|^2}{1-|T|^2}.$$

Thus the conductivity vanishes when $T(\lambda) = 0$. In particular, neglecting the analog of "chemical shifts" γ_{00}, γ_{11} caused by the joining of the cluster to the quantum wire we get:

$$T(\lambda) = \frac{\frac{ik\hbar^2}{m}|\gamma_{01}|^2}{\frac{ik\hbar^2}{m}|\gamma_{01}|^2 + Q(\lambda)}, \quad \lambda = k^2.$$

We see that the conductivity of the device considered vanishes for electrons having the energies equal to ones of the non-occupied orbitals corresponding energy levels α_s of the attached cluster. In particular, if the cluster is in the ground state, $A = A_g$, and the non-occupied energy levels are α_e, α_1, α_2, ..., then the transmission coefficient vanishes for electrons with the corresponding energies. If it is in the excited state $A = A_e$, then the nonoccupied levels are equal to . α_g α_1 α_2, hence the transmission coefficient vanishes for electrons having these energies.

If the Fermi level λ_F in the wire coincides with α_e, then in the first case the device conductivity vanishes at cryogen temperature, and it is positive in the second case:

$$\sigma_g = 0,$$

$$\sigma_e = \frac{e^2}{\hbar^2}\frac{|T_e(\lambda_F)|^2}{|T_e(\lambda_F)|^2 - 1},$$

where T_e is the transmission coefficient corresponding to the excited cluster.

The switching on and off of this device can be managed by any type of optical excitations. When excited by the resonance light, the cluster electron is transferred from the level α_g to the level α_e and is supposed to remain there until the next exposition with resonant light induces the inverse transition.

At higher temperature the considerable part of conductivity electrons has the energy λ that differs from λ_F, so the real conductivity should be calculated as a mean value of conductivity $\sigma(\lambda)$ with Fermi distribution $\rho(\lambda, t)$ as follows:

$$\int \sigma(\lambda)\mathrm{d}\rho(\lambda, t) = \bar{\sigma}(t).$$

Obviously the operating of the described gate is not efficient for higher temperatures, since the value of the mean conductivity could be far from zero in ground state. But being joined in a chain, these gates seem to be essentially more efficient even for higher temperatures.

3. Soluble model for optically simulated metal-dielectric transition in infinite quasioned-imensional lattice. In this section we consider the infinite chain of model molecular clusters, similar to one discussed above. We assume, that the clusters are chosen such that in the ground state all of them have the same Hamiltonians

$$A^s = A^s_g = A_g$$

represented by the finite-dimensional operators (diagonal matrices) in the spaces $E^s = E$. Further we assume that the optical excitation with the frequency ν is in resonance with odd clusters only, hence only clusters with the odd numbers $s = 2l + 1$ get excited,

$$\alpha_e^{2l+1} - \alpha_g^{2l+1} = 2\pi\hbar\ \nu,$$

and all excited clusters are equivalent, $A_e^{2l+1} = A_e^1$. Thus, if in the ground state the chain of clusters has the period L, then in the excited state it has the period $2L$. At last we assume that the deficiency

elements $h = h_s$ and the self-adjoint boundary conditions describing the connection of neighboring clusters are the same for all clusters of the chain:

$$\xi_-^s = \gamma\xi_+^{s-1} + \bar{\gamma}\xi_+^{s+1}.$$

We consider a selfadjoint operator $\mathcal{A}_\gamma$ defined in the space $\mathcal{E} = l_2(E)$ of all infinite sequences U^s of E-vectors:

$$U = \{U^s\}_{s=-\infty}^{s=\infty} \subset \mathcal{E} = \sum \oplus E_s.$$

Writing down each component in a form parametrised by the boundary values, as it was done in the previous section

$$U^s = U_0^S + \frac{A^s}{A^s - iI}\ \xi_+^s h + \frac{1}{A^s - iI}\ \xi_-^s h$$

we define the operator by the formula

$$(\mathcal{A}_\gamma U)^{(s)} = A^s U_0^s - \frac{1}{A^s - iI}\ \xi_+^s h + \frac{A^s}{A^s - iI}\ \xi_-^s h$$

and the proper translation invariant self-adjoint boundary conditions imposed onto the boundary values $\xi_\pm^s$:

$$\gamma\xi_+^{s-1} + \bar{\gamma}\xi_+^{s+1} = \xi_-^s.$$

Then the operator $\mathcal{A}_\gamma^g$ is the one-particle lattice model with the period L, and the operator $\mathcal{A}_\gamma^e$ is the lattice model with the period $2L$. In the generic case the spectrum of the operator $\mathcal{A}_\gamma^g$ consists of the $\dim A_g$ bands which are determined by the solutions of the algebraic equation:

$$Q_g(\lambda) = \langle \frac{I + \lambda A_g}{A_g - \lambda I} h, h\rangle = \gamma\theta^{-1} - \bar{\gamma}\theta,$$

with the uni-modular unknown function $\theta = \mathrm{e}^{i\kappa}$, κ playing the role of quasimomentum exponential $e^{i\kappa}$, and

$$U = \{U^s\} = \left\{U^0\theta^s\right\}$$

generally playing the role of Bloch-type solutions of the corresponding homogeneous equation and the role of eigenfunctions of $\mathcal{A}_\gamma^g$ on the corresponding spectral bands. The condition of existence of nontrivial bounded solutions of the last algebraic equation takes the form

$$|Q_g| \equiv \left|\langle \frac{I + \lambda A_g}{A_g - \lambda I} h, h\rangle\right| \leq 2|\gamma|.$$

The spectrum of the operator $\mathcal{A}_\gamma^g$ consists of spectral bands, constituted by the (real) values of the energy λ, which satisfy the last condition. Two Bloch eigenfunctions correspond to each value λ from the band:

$$\Psi_\pm^s = \frac{A^g + iI}{A^g - \lambda I} L\theta^{\pm s}, \quad s = 0, t, \ldots.$$

According to the conventional quantum-mechanical interpretation the electrons in the Bloch states, corresponding to spectral bands of nonexcited chain are not "localized" but are "moving" in the infinite one-dimensional conductor formed by the periodic chain of clusters in the ground state. Under the values λ, lying outside of the spectrum $|\theta(\lambda)| < 1$ or $|\theta(\lambda)| > 1$, the corresponding Bloch solutions $\Psi_\pm$ are exponentially decreasing in one direction and exponentially growing in the opposite one so they can't be eigenfunctions of the continuous spectrum. In real lattices the electrons with the corresponding energies are either absent or localized on impurities in the proper bound states,which are combined of the decreasing branches of the corresponding Bloch solutions.

If each odd cluster is excited, and each even one is in the ground state

$$A^{2l} = A_g,$$

$$A^{2l+1} = A_e,$$

then the corresponding Hamiltonian $\mathcal{A}_\gamma^e$ is also self-adjoint one, and its spectrum also has a band structure. However, the condition of belonging λ to the spectrum of the $2L$-periodic lattice is described

technically in other form. Now the role of the period of the unperturbed lattice operator is played by the orthogonal sum $A_g \oplus A_e$ in $E \oplus E$, and the Bloch-vector of the perturbed lattice with the boundary conditions switched on is represented as a sequence of two-component E-vectors

$$\Psi = \{\theta^n \begin{pmatrix} v_0 \\ v_1 \end{pmatrix}\}.$$

Denoting by $A^*_{e,g}$ the formal expression for the operator's action on elements of E, represented as in the first section,

$$U_1 = U_{10} + \frac{A}{A - iI}\xi_+ \cdot h + \frac{1}{A - iI}\xi_- \cdot h,$$
$$(A - iI)U_{10} \perp h,$$

we write down the corresponding homogeneous equation for the boundary values $\xi_+, \xi_- = Q(\lambda)\xi_+$ of Bloch vectors of the exited chain

$$\Psi_\pm = \left\{ \begin{array}{c} \frac{A_g+iI}{A_g-\lambda I}\xi^g_+ \\ \frac{A_e+iI}{A_e-\lambda I}\xi^e_+ \end{array} \theta^{\pm l} \right\}_{l=-\infty}^{l=+\infty}.$$

in the following form

$$\left[\begin{array}{cc} Q_g(\lambda) & -\bar\gamma - \gamma\bar\theta \\ -\gamma - \bar\gamma\theta & Q_e(\lambda) \end{array} \right] \left(\begin{array}{c} \xi_g \\ \xi_e \end{array} \right)_+ = 0,$$
$$\left[\begin{array}{cc} Q_g(\lambda) & -\bar\gamma - \gamma\theta \\ -\gamma - \bar\gamma\bar\theta & Q_e(\lambda) \end{array} \right] \left(\begin{array}{c} \xi_g \\ \xi_e \end{array} \right)_- = 0.$$

In particular, from the second equation we have the following condition for the corresponding quasi-momentum exponential $\theta = e^{i\kappa}$

$$Q_g(\lambda)Q_e(\lambda) = 4|\gamma|^2 cos^2(\varphi + \frac{\kappa}{2}).$$

Here $\varphi = \arg\gamma$. Thus $cos^2(\varphi + \frac{\kappa}{2}) = \pm\frac{\sqrt{Q_g Q_e}}{2|\gamma|}$, and

$$\xi^-_g = \frac{1}{\sqrt{|Q_g|}},\ \xi^-_e = \frac{e^{i\kappa}}{\sqrt{|Q_e|}}.$$

It follows from here, that the spectral bands of the excited lattice coincide with the intervals of real axis, where $0 \le Q_g(\lambda)Q_e(\lambda) \le 4|\gamma|^2$. Another important fact concerning the boundary values $\xi^e_{g,e}$ of Bloch vectors will be used in the following section for estimates of the transmission coefficient:

The linear combination of the boundary values with pure imaginary coefficient k:

$$\xi^-_g + ik\gamma\theta\xi^-_e$$

does not have roots on the real axis λ.

Assuming that the spectral properties of clusters in the ground and excited states are the same as in the previous section we see that the functions Q_g, Q_e are essentially distinguished by the position of one pole only:

$$\frac{1 + \alpha^2_e}{\alpha_e - \lambda}|\langle h, \phi^e\rangle|^2 \longleftrightarrow \frac{1 + \alpha^2_g}{\alpha_g - \lambda}|\langle h, \phi^g\rangle|^2.$$

This leads to the partition of the lower spectral band of the L-periodic chain of clusters A_g into two subbands corresponding to the $2L$-periodic chain of A_g, A_e-clusters. The arising lacuna (spectral gap) δ is found from the condition:

$$Q_e(\lambda)Q_g(\lambda) < 0,$$

and shifts $\lambda^\pm_e \to \lambda^\pm$ of the upper and lower bounds are determined from the equation:

$$Q_e(\lambda)Q_g(\lambda) = 4|\gamma|^2.$$

If the residues $(1+\alpha^2)|\langle h, \phi^e\rangle|^2$ at the poles α_e α_g, which correspond to the ground and excited states of the clusters, are approximately equal, then the dispersion curves $\lambda = \lambda(\kappa)$ corresponding to the excited and the nonexcited chain are approximately parallel and hence the lacuna (spectral gap) width $|\delta|$ proves to be approximately equal to the distance between the ground and exited energy levels of odd clusters:

$$\delta \sim \alpha_e - \alpha_g.$$

The described chain exhibits a remarkable type of behavior under resonance optical excitations, which can be interpreted as a "*Simulated Mott-Pejerls transition*". If the Fermi level λ_F is situated at the center of the gap δ (thus *inside* the conductivity band of the chain in ground state), then the chain in the ground state is equivalent to one-dimensional metallic conductor. On the other hand the Fermi level is situated inside the gap δ of the exited chain, hence the *exited chain is a dielectric one for electrons on Fermi level* λ_f. This is exactly Mott-Pejerls-type behavior, see [19]. It is important, that the chain remains dielectric within some interval of energies near λ_f, defined by the width of the gap $|\delta|$, hence the described chain *can plays the role of the gate in some interval of temperatures* $0 \le T \le \frac{|\delta|}{2k}$. Under conditions above this interval is approximately determined by the distance between the levels $\alpha_g - \alpha_e$. In section 2 the advantages of narrow-band semiconductors were discussed for creating quantum wires with large values of de Broghlie wave length. Here we underline another essential advantage of the the narrow-gap semiconductors with small values m : they manifest a high resolution of the levels in quantum well which can exceed kT already in the range of room temperatures. It means, that the distance between energy-levels of cluster orbitals is large , and thus, according to observation above, the critical temperature $\frac{|\delta|}{2k}$ may be significantly higher than the helium temperature or even higher, then the nitrogen one.

4. Scattering by finite chain of clusters. The quantum gate can't be technologically implemented in the form of infinite cluster chain. We consider now the finite chain of clusters length $N\ L = 2n\ L$ inserted into a quantum wire. Assuming that the clusters of the chain possess properties described in the previous section, we solve the scattering problem for exited chain and for the chain in ground state. The corresponding transmission coefficient proves to be exponentially small for large N outside the spectral bands of the exited infinite chain, but is close to the transmission coefficient "through the semi-infinite chain" in the ground state. Practically it means that the finite chain inserted in the quantum wire can serve as a quantum gate under certain conditions on the parameters of the clusters and the chain.

We construct the model Hamiltonian of a single electron on the quantum wire with the inserted finite lattice by means of extension theory methods of two components: the free Hamiltonian on the wire and lattice Hamiltonian on the inserted periodic chain with proper boundary conditions at the points of contacts:

$$\begin{pmatrix} 0 & \bar\gamma & 0 & 0 & ... & ... & ... & 0 & 0 & 0 \\ \gamma & 0 & \bar\gamma & 0 & 0 & ... & ... & ... & 0 & 0 \\ 0 & \gamma & 0 & \bar\gamma & 0... & ... & ... & ... & 0 & 0 \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & \gamma & 0 & \bar\gamma & 0 & 0 \\ ... & ... & ... & ... & ... & ... & \gamma & 0 & \bar\gamma & 0 \\ ... & ... & ... & ... & ... & ... & ... & \gamma & 0 & \bar\gamma \\ ... & ... & ... & ... & ... & ... & ... & ... & \gamma & 0 \end{pmatrix} \begin{pmatrix} u'(0) \\ \xi_g^0 \\ \xi_e^0 \\ \xi_g^1 \\ ... \\ ... \\ \xi_e^{n-1} \\ \xi_g^n \\ \xi_e^n \\ -u'(NL) \end{pmatrix} = \begin{pmatrix} u(0) \\ Q_g\xi_g^0 \\ Q_e\xi_e^0 \\ Q_g\xi_g^1 \\ ... \\ ... \\ Q_e\xi_e^{n-1} \\ Q_g\xi_g^n \\ Q_e\xi_e^n \\ u(NL) \end{pmatrix}.$$

The scattered waves are combined of the solutions of the stationary Schrödinger equation on the quantum wire

$$\begin{array}{ll} Te^{ikx}, & -\infty < x \le 0, \\ e^{ikx} + Re^{-ikx}, & N\,L \le x < \infty, \end{array}$$

and Bloch solutions on the inserted lattice $0 \le l \le N$:

$$\Psi = \alpha\Psi_+ + \beta\Psi_-.$$

A straightforward calculation gives us the connection between α and β:

$$\frac{\beta}{\alpha} = -\frac{\theta^{-1}\xi_e^+ - ik\gamma\xi_g^+}{\theta\xi + g^- - ik\gamma\xi_g^-},$$

and the explicit expression for the transmission coefficient. Let us denote

$$\Delta_+, \equiv \frac{\theta\xi_g^+ + ik\gamma\xi_e^+}{\theta^{-1}\xi_e^+ - ik\gamma\xi_g^+}, \quad \Delta_- \equiv \frac{\theta^{-1}\xi_g^- + ik\gamma\xi_e^-}{\theta\xi_e^- - ik\gamma\xi_g^-}.$$

Then

$$T = \frac{-2ik\gamma e^{iLNk}}{\theta\xi_e^- - ik\gamma e_g^-}\frac{\xi_g^+\xi_e^-\theta - \xi_g^-\xi_e^+\theta^{-1}}{\theta^n\Delta_+ - \theta^{-n}\Delta_-}.$$

Due to the statement from the previous section the coefficient in front of θ_n in the denominator does not have real zeroes, hence the transmission coefficient has the following asymptotic on spectral gaps of the exited chain for large N:

$$T \approx 2ik\frac{\bar{\gamma}}{\gamma}\frac{e^{ikLN}\theta^n}{\theta^{-1}\xi_g^- + ik\gamma\xi_g^-},$$

so it is exponentially small inside the spectral gaps of the exited chain.

On the other hand, the similar calculation of the reflection coefficient R^N of the chain in the ground state gives

$$R_g^N = e^{2ikLN}\frac{\theta^N\Delta_1 - \theta^{-N}\Delta_2}{\theta^N\Delta_3 - \theta^{-N}\Delta_4},$$

where

$$\Delta_1 \equiv \frac{Q+ik|\gamma|^2-\theta^{-1}\gamma}{Q-ik|\gamma|^2-\theta\bar{\gamma}},$$
$$\Delta_2 \equiv \frac{Q+ik|\gamma|^2-\theta\gamma}{Q-ik|\gamma|^2-\theta^{-1}\bar{\gamma}},$$
$$\Delta_3 \equiv \frac{Q-ik|\gamma|^2-\theta^{-1}\gamma}{Q-ik|\gamma|^2-\theta\bar{\gamma}},$$
$$\Delta_4 \equiv \frac{Q-ik|\gamma|^2-\theta\gamma}{Q-ik|\gamma|^2-\theta^{-1}\bar{\gamma}}.$$

Note that $|\Delta_{1,2}| = 1$, hence the reflection coefficient corresponding to the inserted into quantum wire finite chain of N equivalent non-excited clusters has exactly N roots on each spectral band of the corresponding infinite lattice. Due to the unitarity of the complete scattering matrix it means that the corresponding transition coefficient T_g is modulo one at N spectral points on each spectral band of the corresponding infinite lattice.

The Reflection Coefficient $R_g^N(k)$ is a contracting analytic function on the lower halfplane of momentum k. It can be shown, that on every compact domain of it it is converging uniformly to the reflection coefficient R_g^∞, corresponding to the semi-infinite lattice. ¿From the observation above follows, that this convergence does not take place on real axis of momentum,in particular on spectral bands in the complex plane λ of energy. Nevertheless for any problem for the corresponding nonstationary Schrödinger equation with smooth initial data given the in form of incoming waves in quantum wire one can use the fact, that both reflection coefficients are close "in medium" for large N:

$$R_g^N(k) \approx R_g^\infty.$$

Thus the measure of "formal garbage" produced by any scattering act by finite chain is limited by the corresponding reflection coefficient of the semi-infinite lattice. But similarly to the the situation described in the section 2 we see that the information on the reflected waves is contained actually in the transmitted waves, so it is never lost, it is " potentially observable".

The real garbage in a single act of computation is caused by the measurement of the scattering state, i.e. by projection of the state onto the states of measuring device, or by averaging them over stochastic states of the random background. The loss of this garbage is unrecoverable. The corresponding information is irreversibly lost which makes the computation irreversible. In [18] efficient probabilistic algorithms for classical computations are discussed. Similarly to the discussed quantum computations,

these algorithms are "polynomial-time algorithms". Professor C. Calude formulated the following question: Are there any 'typical features' of quantum computations which make them different, and more efficient, than classical probabilistic computations? Our model permits to compare the work of the described quantum gates with the corresponding classical gates as an element of classical circuit acting in frames of a "random" algorithm. Really, the single act of quantum computation consists in opening or closing the quantum gate. Assuming that the life-time of inner cluster electrons on the excited level is much longer than typical time-intervals of the process under consideration, we see that the the quantum evolution of the conductivity electron is unitary, and the computation is invertible, unless we do not project the result onto the states of the measuring device. *The inversibility of the computation is produced by the act of measurement only.*

If the constructed self-adjoint operator is positive, we can consider it as a generator of evolution of the transition probabilities of some Markov process. Then the relevant parabolic equation is interpreted as a Fokker-Plank equation for transition probabilities. The corresponding evolution is contracting, hence the conservation law is absent, and *the garbage, produced by the process, is killed each moment in the course of evolution, resulting in the global irreversibility of the process.* So the important difference between the quantum computations and similar probabilistic algorithms is the moment when the unrecoverable garbage is produced, which corresponds to the *irreversible* loss of information. For classical computations it is produced *in course of evolution*, and for quantum ones it is produced just in the last moment. The "potentially observable garbage", caused by outgoing waves in quantum process does not destroy the reversibility of the process of quantum computations, though these waves remove some part of wave-packet to infinity. Possibly this difference can help defining the proper domain of applications of both computational techniques.

The implementation of the construction of quantum gates described in section 4 and other constructions based on simulated Mott-Pejerls transitions (see [20]) require solving numerous difficult physical and technological problems such as the choice of proper quasi-molecular clusters and their location inside the isolating medium, the information output/input from the macroscopic level, the choice of the proper optical window for each type of gates etc. Possibly, the most prospective constructions of such kind may be created as polymers or biomolecules. The general advantage of the Mott-Pejerls gates is higher stability of their characteristics and a relatively weak dependence of their working regimes on temperature.

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