Novel *coherent* quantum bit using spatial quantization levels in semiconductor quantum dot

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1   Introduction

Within last decade there has been achieved large progress in theory of quantum computing. Unfortunately the experimental realization of practically valuable quantum computers has not been performed mainly due to lack of scalable coherent controllable two-level quantum systems. Semiconductor nanostructures were considered as a candidates to basic elements of quantum computer — quantum bits (qubits). In 1995 A. Barenco, D. Deutsch, A. Ekert, and R. Jozsa [1] for the first time offered to use as base states ("0" and "1") of qubits two bottom levels of spatial quantization of single-electron quantum dots. To implement two-qubit operations it was suggested to use electrical dipole interaction. Soon the same authors (A. Ekert and R. Jozsa) [2] evaluated coherence of such systems and proved that ordinary quantum dots are too incoherent to be quantum bits. The variants of such structures were investigated by other authors in papers [3, 4]. Potential confining at least one of these quantum dots was assumed asymmetrical. Distance between the bottom levels was about 10–100 meV.

Our proposal is to use mesoscopic structures with small (below 1 meV) separation between energies of two bottom states. The work frequency of such structures, which is proportional to energy separation, is surely to be decreased compared to early proposed ones. But processes of spontaneous emission of photons and phonons are proportional to polynom (cubic or higher degree) of energy of transition. Therefore errors rate per one implemented quantum operation is to be smaller compared to common structures.

2   Structure and principles of operation

In the proposed structure we offer to use as a qubit a quantum dot with a symmetrical potential profile, as shown in Figs. 1, 2. The presence of two minima of potential separated by a thick barrier is essential. In a quantum dot there is one electron. The presence of the second electron is energetically unprofitable because of Coulomb interelectron repulsion. Although the qubit proposed can be made in principle of any semiconductor for technological reasons we focus our attention on GaAs/AlGaAs structures because this material proved to reliable basis for observation of various coherent quantum effects. In GaAs quantum

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dots at distance between minima $r = 10\,\mathrm{nm}$ (see Fig. 3) the Coulomb energy is about $e^2/\kappa r = 11\,\mathrm{meV}$, that allows to exclude a spontaneous charging of a dot by the second electron.

To find work frequencies and other working parameters of an offered qubit, two-dimensional Schrödinger equation for an electron in a quantum dot in GaAs with model potential V (shown on Fig. 2) was solved numerically:

$$V = \frac{m\omega^2(x^2 + y^2)}{2} + V_B \exp\left[-\frac{x^2}{(wl)^2}\right],\tag{1}$$

where $m = 0.065 m_e$; $l = 20\,\mathrm{nm}$; $V_B = 1.5 \cdot 10^{-19}\,\mathrm{J}$; $w = 0.08 \div 0.34$ ($r = 11 \div 34\,\mathrm{nm}$).

The obtained wavefunctions of four bottom states of an electron for this potential are shown in Figs. 4–7. Two bottom energy levels of an electron in such point correspond to wavefunctions Ψ_1 (Fig. 4) and Ψ_2 (Fig. 5). For logic "0" and "1" it is convenient to take the normalized sum and difference of Ψ_1 and Ψ_2 rater than states with the certain energy:

$$|0\rangle = \frac{1}{\sqrt{2}}\left(\Psi_1 + \Psi_2\right), \qquad |1\rangle = \frac{1}{\sqrt{2}}\left(\Psi_1 - \Psi_2\right).\tag{2}$$

The given states correspond to almost complete localization of an electron in one of minima of potential, as shown in a Figs. 8, 9. It allows to implement write of the input data and reading of results by methods of single-electronics with the help of the read-out gates, as shown in a Fig. 1. The central gate (control gate) serves for downturn of a potential barrier while implementing quantum unitary transformations, as will be shown below.

2.1 Implementation of one-qubit unitary operations

In the beginning qubit is not affected by operations and it is in the state

$$\Psi(0) = c_0 |0\rangle + c_1 |1\rangle.\tag{3}$$

Electron wavefunction evolve according to Schrödinger equation

$$i\hbar \frac{d\Psi}{dt} = H\Psi,\tag{4}$$

where Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta + V,\tag{5}$$

where V is given by (1).

Different voltages on the control gate correspond to different barrier heights V_B. Therefore energies of the ground and first excited state also depend on V_B. $\left(\hbar\omega_{1,2} = \hbar\omega_{1,2}(V_B)\right)$. When barrier is high, the energy levels of two bottom states practically merge so two bottom levels evolve with the common frequency ω:

$$\Psi(t) = e^{-i\omega t} \left(c_0 \left| 0 \right\rangle + c_1 \left| 1 \right\rangle \right). \tag{6}$$

The downturn of a barrier results in an inequality of frequencies ($\Delta\omega = \omega_2 - \omega_1 > 0$) and to periodic rotation of vector of state of qubit in basis ($\left| 0 \right\rangle, \left| 1 \right\rangle$).

$$\Psi(t) = \frac{1}{\sqrt{2}} \left(c_0 + c_1 \right) \Psi_1 e^{-i\omega_1 t} + \frac{1}{\sqrt{2}} \left(c_0 - c_1 \right) \Psi_2 e^{-i\omega_2 t}, \tag{7}$$

that is

$$
\begin{aligned}
\Psi(t) &= e^{-i(\omega_1 + \omega_2)t/2} \big[(c_0 \cos \Delta\omega t/2 + i\, c_1 \sin \Delta\omega t/2) \left| 0 \right\rangle + \\
&\quad + (c_1 \cos \Delta\omega t/2 + i\, c_0 \sin \Delta\omega t/2) \left| 1 \right\rangle \big].
\end{aligned}
\tag{8}
$$

Having applied a pulse of a positive voltage of the certain duration t_{NOT}, equal to $\pi/\Delta\omega$, we (an insignificant common phase factor $\exp\left[-i\pi\omega_1/(\omega_2 - \omega_1)\right]$ can be neglected) shall transfer a state of a qubit (3) into a state (as shown in Fig. 10):

$$\text{NOT}(\Psi_0) = c_1 \left| 0 \right\rangle + c_0 \left| 1 \right\rangle. \tag{9}$$

So, with the help of the given procedure it is possible to exchange amplitudes at "0" and "1", that is to carry out unitary NOT operation. Changing the duration of a pulse it is possible to carry out rotation of qubit state to any required angle.

2.2 CNOT gate implementation

For construction of the universal quantum computer it is also necessary to be able to realize at least one nontrivial (not decomposable into a sequence of one-qubit gates and permutations) two-qubit operation. We consider realization of CNOT operation. (Depending on state of control qubit, on target qubit should be carried out either operation of identity or NOT). For implementation of the CNOT gate between the neighbour qubits the Coulomb interaction is used. We arrange two qubits as shown in a Fig. 3. To exclude exchange effects it is supposed that the qubits are separated by completely opaque barrier. Then Hamiltonian of electron in target qubit becomes

$$H_t = -\frac{\hbar^2}{2m}\Delta + V + V_C, \tag{10}$$

where Coulomb potential due to electron in control qubit

$$V_C(x, y) = \iint du\, dv\, \frac{\left| \Psi_C(u, v) \right|^2 e^2}{\kappa \sqrt{(x + v)^2 + (y + R - u)^2}}, \tag{11}$$

where $\Psi_C(u, v)$ is a wavefunction of electron in control qubit, u, v are coordinates in coordinate system of control qubit, e is the electron charge and R is a

separation between qubits' centers. Height of barrier dividing the right (target) qubit depends on state of the left (control) qubit. The addition to the height of barrier of the target qubit can be roughly estimated in the following way: when control qubit is in state $|0\rangle$ or $|1\rangle$ we can assume that electron is a point charge located in electron density maximum. Then the Coulomb potential in the barrier dividing target qubit will be

$$V_C\left(0, y\right) = e^2 / \kappa\left(y + R + s\,r/2\right), \tag{12}$$

where s corresponds to state of control qubit: $s = 1$, when control qubit is in state $|0\rangle$, and $s = -1$, when control qubit is in state $|1\rangle$.

In such structure CNOT gate can be implemented as follows. Having slightly opened the barrier in a target qubit with the help of its control gate it is possible to achieve application to the target qubit the operation of identity, when the control qubit is in a state $|0\rangle$ and operation NOT, when the control qubit is in a state $|1\rangle$, that is operation CNOT. Consider a case, when the control qubit is in one of base states. Because of Coulomb influence of a control qubit on height of a barrier in a target qubit the duration of the NOT operation in these cases will differ ($t_{NOT0} \neq t_{NOT1}$). Duration of a pulse on a gate of a target qubit we choose in the following way:

$$t_{CNOT} = t_{NOT0}\,t_{NOT1}/(t_{NOT1} - t_{NOT0}). \tag{13}$$

Varying amplitude of a pulse we shall achieve, that the ratio

$$t_{NOT1}/2(t_{NOT1} - t_{NOT0}) \tag{14}$$

will be an integer (it is the large value, as in our case interaction is weak, so by small change of amplitude we attain the nearest integer value)

$$t_{NOT1}/2(t_{NOT1} - t_{NOT0}) = N. \tag{15}$$

If the control qubit is in state "0", then the action of a pulse is equivalent to consecutive application of *even* $(2N)$ of number of operations NOT to the second qubit, that is operation of identity. If the control qubit is in state "1", then the action of a pulse is equivalent to consecutive application of *odd* $(2N-1)$ number of operations NOT to the second qubit, that is NOT operation.

While modelling the interaction was calculated directly by the Coulomb's law (in all cells of a two-dimensional grid the field created by a partial charge of a control qubit form all cells) was calculated. Exchange effects were neglected. The dependencies of minimal durations of operations NOT and CNOT depending on geometrical parameters are shown in Fig. 11, 12.

3 Numerical modeling

For calculation the method of simple iterations was used. Potential should be symmetrical and have 2 minima, that means presence of a barrier between these

minima. Similar potential for a two-electronic quantum dot was used in [5]: he has offered to use polynomial potential of the 4-th order like

$$V(x,y) = \frac{m\omega^2}{2}\left(\frac{1}{4a^2}\left(x^2 - a^2\right)^2 + y^2\right) \tag{16}$$

with minima in points $\pm a$.

In this work as potential of a quantum dot with the built-in tunnel barrier was used potential (1). Such potential can be varied by changing the following parameters: l (characteristic size of a qubit ($\sim 20\,\text{nm}$)), V_B (height of a barrier ($\sim 1\,\text{eV}$)) and w (the width of a barrier in relation to l (~ 0.1)). Varying values of these parameters, it is possible to tune the characteristics of structure.

Consider an electron strongly limited in a direction, perpendicular to a surface of a heterojunction. Thus distances between levels of spatial quantization (2D electron gas subbands) in this direction is about $100\,\text{meV}$. At low temperatures and weak influences the electron remains in the bottom subband. Thus its motion can be considered as two-dimensional, and the wavefunction of an electron is factorized into

$$\Phi(x,y,z) = \Psi(x,y)\,g(z). \tag{17}$$

For wavefunction $\Psi(x,y)$ we have solved 2D Schrödinger equation with the potential V using simple iterations method with orthogonalization on each iteration. We have modelled an area $60 \times 40\,\text{nm}^2$ using mesh with the same step in both directions 0.5 nm. We have iterated 4 bottom state wavefunctions controlling their orthogonality. The mean number of iterations was about 10000. To find energies of states of an electron, the mean value of an energy for a wavefunction Ψ under the formula $\langle\Psi|\,H\,|\Psi\rangle$, where H is the operator of Hamilton with real potential was calculated. After that the program show us the diagram of the bottom part of a spectrum of system, and also frequency of transitions from the exited energy levels on basic. These frequencies were also used in research of processes of decoherence in structure. Besides half of time of transition from the first exited level on basic and back also was accepted for the minimal time of operation of the NOT gate.

For the nontrivial two-qubit CNOT gate it is necessary to include interaction between control and target qubits. In studied structure the electrical (mostly dipole) interaction is used. For this purpose we arrange a target qubit about an end face of a control qubit, having turned it on 90 degrees in a plane of structure. At such arrangement a state of an electron in a control qubit (the electron is farther or closer to the middle of a target qubit) effectively reduces or increases height of a barrier in a target qubit, that changes time of operation of the NOT gate. As the points of localization of an electron in a target qubit are located symmetrically in relation to the control qubit, so the change of a state of a target qubit does not render influence in the first order on a state of a control qubit.

For calculation of interaction it is necessary to calculate potential created by an electron of a control qubit in the field of a target qubit. For this purpose

it is possible to take advantage of two methods: solution of a Poisson equation or calculation of an electrostatic field using Coulomb's law. The second method was used. For this purpose it was supposed, that in each node of a mesh in the area of a control qubit there is a point charge, which value is equal to value of a charge of an electron multiplied on a value of function of spatial distribution of an electron at this node of a mesh. As function of distribution it is natural to take a square of the module of a wavefunction. As the function of distribution is normalized, this operation simply represents an electron by system of point charges with a cumulative charge equal to a charge of an electron.

The durations of the NOT gate for two extreme states of an electron in a control qubit were obtained: when the electron wholly is in most distant from a target qubit and when the electron wholly is near to a target qubit. Knowing these times, it is possible to calculate duration of operation of the CNOT gate.

4 Coherence of structure

Significant difficulty interfering creation of the large scale quantum computer is the problem of decoherence of a quantum state because of interaction with an environment bringing in errors. It is proved [6], that if the decoherence occurs slowly enough, that, in particular, means, that at calculation occurs no more than δ failures for one computing step (by various estimations δ should lie in a range from 10^{-2} to 10^{-5}), with the help of special error correcting algorithms and codes demanding polynomial increase of computing expenses, modeling functioning of ideal (coherent) quantum computer and steady implementation of any quantum algorithm is possible.

While calculating the decoherence in offered structure the low-temperature limit ($T \to 0$) was considered. The given approximation is justified, as the modern cryogenic engineering allows to carry out functioning nanoelectronic structures at temperatures down to several millikelvins, that is sufficiently lower than the distance between bottom and first excited levels. The case of high temperatures represents only academic interest because of inevitable fastest decoherence and impossibility of correct work of the quantum computer. However, in solid-state structures even at absolute zero of temperature the processes of decoherence owing to spontaneous emission of photons or acoustic phonons with transition of an electron from excited to the basic level are possible. These processes will determine the degree of coherence in our structure. We separately investigated spontaneous emission of photon, of deformation acoustic phonon and of piezoelectric acoustic phonon.

4.1 Emission of photon

Consider process of decoherence through emission of photon. The transition from first exited on the basic level is dipole. The probability of dipole transition

is given by the known formula [7]

$$W_{Ph} = \frac{4\omega^3}{3\hbar c^3} |\mathbf{d}|^2, \tag{18}$$

where the dipole moment

$$\mathbf{d} = \int d^2 r \, \Phi'(\mathbf{r})^* \, e\mathbf{r} \, \Phi(\mathbf{r}). \tag{19}$$

From the symmetry of wavefunctions it follows that of a component d_y will be zero, and x-component can be calculated through integral not on all space, but only on half-space $x > 0$:

$$d_x = 2 \int\limits_{x>0} dx \, dy \, \Phi'(\mathbf{r})^* \, ex \, \Phi(\mathbf{r}). \tag{20}$$

As the integrand at large r exponentially decreases with increasing of x, integral can approximately be evaluated, having reduced integration on half-space to integration on area $0 < x < x_{max}$. To estimate this integral we can replace x in an integrand with its maximal value, i.e.

$$d_x \le 2ex_{\max} \int\limits_{0<x<x_{\max}} dx \, dy \, \Phi'(\mathbf{r})^* \, \Phi(\mathbf{r}), \tag{21}$$

and as the wavefunctions on area of integration practically coincide, integral will be equal to $1/2$, as the integration is made on half-space, and integral on all space from a condition of a normalization of wavefunctions is equal to 1. In our case of wavefunctions have on $x > 0$ maxima in some point r, behind which exponentially fall down, and as x_max it is enough to choose $2r$. Then $d_x \le 2er$, hence estimation for probability of spontaneous emission of photon to look like

$$W_{Ph} \le \frac{16\varepsilon_{10}^3 e^2 r^2}{3\hbar^4 c^3}. \tag{22}$$

4.2   Emission of acoustic phonon

The probability of relaxation from the excited state to the ground one, by emission of acoustic phonon, is calculated by formula:

$$w_{10} = \frac{2\pi}{\hbar} |M|^2 \delta(\varepsilon_{10} - \hbar sq), \tag{23}$$

where $M = \langle f| T |i\rangle$ ($|i\rangle$ is the initial state (the electron is in the excited state with an energy ε_1), $|f\rangle$ is the final state (the electron is in the base state with an energy ε_0, $\varepsilon_{10} \equiv \varepsilon_1 - \varepsilon_0$, the phonon carried away an energy $\hbar sq$), T is the transition operator) is the matrix element of transition appropriate to emission of phonon, s is the speed of sound ($5.2 \cdot 10^3$ m/s in GaAs), $\mathbf{q}$ is a wave vector of the phonon.

Disturbance created by one phonon $s\mathbf{q}$ [8]:

$$V_{s\mathbf{q}} = \frac{1}{L^{3/2}} \left[\frac{\hbar a_0^3}{2M_0 \omega_{s\mathbf{q}}} \right]^{1/2} e^{i\mathbf{q}\mathbf{r}} v_{s\mathbf{q}}(\mathbf{r}), \tag{24}$$

and

$$v_{s\mathbf{q}}(\mathbf{r}) = \sum_{\mathbf{a}\alpha} V_{\mathbf{a}\alpha}(\mathbf{r}) \, \mathbf{d}_{s\mathbf{q}}^{\alpha} e^{i\mathbf{q}(\mathbf{a}-\mathbf{r})}, \tag{25}$$

where M_0 is the mass of an elementary cell, a_0^3 is the volume of an elementary cell, d is a unitless vector of polarization orthonormalized by the condition

$$\sum_{\alpha} M_{\alpha} \left(\mathbf{d}_{s\mathbf{q}}^{\alpha} \right)^* \mathbf{d}_{s'\mathbf{q}'}^{\alpha} = M_0 \delta_{s\mathbf{q},s'\mathbf{q}'}, \tag{26}$$

where M_{α} is a mass of atom α. From a normalization follows, that for acoustic phonons at $\mathbf{q} \to 0$ all atoms in a cell are displaced equally:

$$\mathbf{d}_{s\mathbf{q}}^{\alpha} = \mathbf{d}_{s\mathbf{q}}, \qquad \left| \mathbf{d}_{s\mathbf{q}} \right| = 1. \tag{27}$$

It is convenient to define a total probability of emission of phonon, i.e. probability to emit though any phonon, considering, that the crystal is limited to a normalizing volume L^3, and the allowable values of a pulse are quasidiscrete. Then the probability of transition is probability that in unit of time electron will make a transition from one quasidiscrete state in another; the dimensional representation of it is s^{-1}. The certain thus probability depends on a normalizing volume. Probability of transition of an electron from the given state

$$W = \sum_{\mathbf{q}} w_{\mathbf{q}}. \tag{28}$$

As the allowable values of q are located very richly, on distance $2\hbar/L$, it is possible to pass from a summation on $\mathbf{q}$ to integration by a rule

$$\sum_{\mathbf{q}} (\ldots) = L^3 \int \frac{d^3 q}{(2\pi)^3} (\ldots). \tag{29}$$

Then

$$W = L^3 \int \frac{d^3 q}{(2\pi)^3} w_{10}. \tag{30}$$

4.3 Emission of piezoelectric acoustic phonon

In 1961 A.R. Hutson considered interaction of electrons and acoustic waves due to piezoelectric effect [9]. The matrix element of interaction of an electron with an electromagnetic field is given by the formula

$$M_{PA} = \int d^3 r \, \Phi'(r)^* \, e\varphi(r) \, \Phi(r), \tag{31}$$

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where $\Phi(r)$ is wavefunction of an initial state of electron $|i\rangle$, $\Phi'(r)$ - of the final state $|f\rangle$, $\varphi(r)$ is the macrofield created by a phonon. It can be found from the Poisson equation

$$\nabla^2 \varphi = 4\pi \operatorname{div} \mathbf{P}, \tag{32}$$

where $\mathbf{P}$ is a dipole moment of unit of volume arisen at deformation of lattice. Use of the Poisson equation instead of complete system of the equations of the Maxwell corresponds to the indefinitely large speed of light c. This assumption is justified, as c is much greater of phase speed ω/q of phonons, that are interesting for us.

At homogeneous acoustic deformation

$$P_j = \beta_{jkl} u_{kl}, \tag{33}$$

where β - piezoelectric constants. Having substituted (33) into (32), it is possible to find a field φ. If we are interested in a field $\varphi_{s\mathbf{q}}$, created by single phonon $s\mathbf{q}$, from the Poisson equation we have

$$\varphi_{s\mathbf{q}} = -i(4\pi/q^2)\mathbf{q}\mathbf{P}_{s\mathbf{q}}, \tag{34}$$

where $\mathbf{P}_{s\mathbf{q}}$ is a polarization created by one phonon $s\mathbf{q}$.

As a result for acoustic phonons it turns out [8]

$$\varphi(\mathbf{r}, t)_{s\mathbf{q}} = \frac{1}{L^{3/2}} \left[\frac{\hbar a_0^3}{2 M_0 \omega_{s\mathbf{q}}} \right]^{1/2} e^{i\mathbf{q}\mathbf{r} - i\omega_{s\mathbf{q}} t} \beta_{s\mathbf{q}} + c.c., \tag{35}$$

where the effective piezoelectric constant of wave $s\mathbf{q}$ is entered:

$$\beta_{s\mathbf{q}} = 4\pi e_i e_k \beta_{ikj} d_{s\mathbf{q}}^j, \qquad e = \mathbf{q}/q; \tag{36}$$

it depends only on a direction of phonon propagation and from a polarization. Thus, the probability to emit a piezoelectric acoustic phonon

$$w_{10} = \frac{\pi \hbar}{\rho \varepsilon_{10} L^3} \left(e\beta_{s\mathbf{q}}\right)^2 |I(\mathbf{q})|^2 \delta\left(\varepsilon_{10} - \hbar s q\right), \tag{37}$$

where

$$I(\mathbf{q}) = \int d^2 r \, \Phi'(\mathbf{r})^* \, \Phi(\mathbf{r}) \, e^{i(q_x x + q_y y)}. \tag{38}$$

With the account of (37) for a total probability we finally have

$$W_{PA} = \frac{\pi \hbar}{(2\pi)^3 \rho \varepsilon_{10}} \int d^3 q \, (e\beta_{s\mathbf{q}})^2 \, |I(\mathbf{q})|^2 \, \delta\left(\varepsilon_{10} - \hbar s q\right). \tag{39}$$

For calculation of probability it is convenient to pass to spherical coordinates. This transition was carried out by a rule

$$\begin{cases} q_x = q \cos\theta \cos\varphi, \\ q_y = q \cos\theta \sin\varphi, \\ q_z = q \sin\varphi. \end{cases} \tag{40}$$

In spherical coordinates the expression for calculation of probability will be

$$W_{PA} = \frac{\pi\hbar}{(2\pi)^3 \rho\varepsilon_{10}} \int d\theta\, d\varphi\, dq\, q^2 \cos\theta\, (e\beta_{s\mathbf{q}})^2 |I(\mathbf{q})|^2 \delta(\varepsilon_{10} - \hbar sq) \qquad (41)$$

We get rid of delta-function under integral, having made integration on dq:

$$W_{PA} = \frac{\pi\hbar}{(2\pi)^3 \rho\varepsilon_{10}} \left(\frac{\varepsilon_{10}}{\hbar s}\right)^2 \frac{1}{\hbar s} \int d\theta\, d\varphi\, \cos\theta\, (e\beta_{s\mathbf{q}})^2 |I(\mathbf{q})|^2. \qquad (42)$$

and finally we get

$$W_{PA} = \frac{\varepsilon_{10}}{8\pi^2 \rho\hbar^2 s^3} \int d\theta\, d\varphi\, \cos\theta\, (e\beta_{s\mathbf{q}})^2 |I(\mathbf{q})|^2. \qquad (43)$$

Vector of displacement of atoms is

$$\mathbf{d} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}. \qquad (44)$$

We consider cubic crystals of symmetry classes O_h and T_d. In crystals O_h with the center of inversion (for example, in Si, as it is possible to show from reasons of symmetry, $\beta = 0$, i.e. the homogeneous deformation does not create macrofields. In crystals T_d without the center of inversion (for example, GaAs) the tensor β_{ikj} has only those components, in which all three indexes i, k, j are various, and all these components are equal. Therefore

$$\beta_{\mathbf{q}} = \frac{4\pi\bar{\beta}}{q^2} (q_x q_y c + q_y q_z a + q_z q_x b), \qquad (45)$$

where $\bar{\beta}$ is constant (e_{14}/κ_0, where e_{14} is sole piezoelectric constant of cubic crystal ($0.16\,\mathrm{C/m^2}$ for GaAs [8, 10]), κ_0 - dielectric permeability (12.8 for GaAs [8, 10])). In next sections we will fulfil calculations of probability of emission of piezoelectric acoustic phonon for GaAs.

4.3.1 Transverse phonons

The phonon with a transverse polarization propagated in any direction, can be decomposed on basis consisting of two polarizations, perpendicular to each other. Choose the first direction of polarization not causing displacement of atoms in direction z. The vector of displacement of atoms for the first direction of polarization also should be perpendicular to the wave vector $\mathbf{q}$ and to be normalized:

$$\mathbf{d}_{T1} = \frac{1}{\sqrt{q_x^2 + q_y^2}} \begin{pmatrix} q_y \\ -q_x \\ 0 \end{pmatrix}. \qquad (46)$$

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For such wave an effective piezoelectric constant

$$\beta_{T1\mathbf{q}} = \frac{4\pi\bar{\beta}}{q^2}\left(-q^2\sqrt{\cos^2\theta}\cos 2\varphi\sin\theta\right) = \tag{47}$$
$$= -4\pi\bar{\beta}\sqrt{\cos^2\theta}\cos 2\varphi\sin\theta,$$

and under integral there will be an expression

$$\left(e\beta_{T1\mathbf{q}}\right)^2 = \left(4\pi e\bar{\beta}\right)^2\cos^2\theta\cos^2 2\varphi\sin^2\theta. \tag{48}$$

The vector of displacement for the second direction of polarization should be perpendicular to the wave vector $\mathbf{q}$, to the vector $\mathbf{d}$ and to be normalized:

$$\mathbf{d}_{T2} = \begin{pmatrix} \frac{q_xq_z}{q_yq}\sqrt{\frac{q_y^2}{q_x^2+q_y^2}} \\ \frac{q_z}{q}\sqrt{\frac{q_y^2}{q_x^2+q_y^2}} \\ -\frac{q_y}{q}\sqrt{\frac{q_x^2+q_y^2}{q_y^2}} \end{pmatrix}. \tag{49}$$

Effective piezoelectric constant for this direction of polarization

$$\beta_{T2\mathbf{q}} = \frac{4\pi\bar{\beta}}{q^2}\left(-\frac{1}{4}q^2\left(\cos\theta + 3\cos 3\theta\right)\cos\varphi\sqrt{\sin^2\varphi}\right) = \tag{50}$$
$$= -\pi\bar{\beta}\left(\cos\theta + 3\cos 3\theta\right)\cos\varphi\sqrt{\sin^2\varphi},$$

and under integral there will be an expression

$$\left(e\beta_{T2\mathbf{q}}\right)^2 = \left(\pi e\bar{\beta}\right)^2\left(\cos\theta + 3\cos 3\theta\right)^2\cos^2\varphi\sin^2\varphi. \tag{51}$$

Summarizing on polarizations of phonons, thus, in the integrand we obtain an expression

$$\left(e\beta_{T\mathbf{q}}\right)^2 \equiv \left(e\beta_{T1\mathbf{q}}\right)^2 + \left(e\beta_{T2\mathbf{q}}\right)^2 = \left(\frac{\pi e\bar{\beta}}{2}\right)^2\cos^2\theta \times \tag{52}$$
$$\times\left(4\left(7 - 9\cos 2\theta\right)\cos 4\varphi\cos^2\theta - 28\cos 2\theta + 9\cos 4\theta + 27\right).$$

Finally, the total probability of emission of phonon with a transverse polarization is given by the following expression:

$$W_{TPA} = \frac{\varepsilon_{10}\left(e\bar{\beta}\right)^2}{32\rho\hbar^2 s^3}\int d\theta\, d\varphi\left|I\left(\varepsilon_{10}\frac{\cos\theta}{\hbar s},\varphi\right)\right|^2\cos^3\theta \times \tag{53}$$
$$\times\left(4\left(7 - 9\cos 2\theta\right)\cos 4\varphi\cos^2\theta - 28\cos 2\theta + 9\cos 4\theta + 27\right).$$

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4.3.2 Longitudinal phonons

The phonon with a longitudinal polarization propagated in some direction, will cause displacement of atoms in the same direction:

$$\mathbf{d}_L = \frac{1}{q} \begin{pmatrix} q_x \\ q_y \\ q_z \end{pmatrix}. \tag{54}$$

Effective piezoelectric constant for such vector

$$\beta_{L\mathbf{q}} = \frac{4\pi\bar{\beta}}{q^3} 3 q_x q_y q_z, \tag{55}$$

and the integral expression will get

$$(e\beta_{L\mathbf{q}})^2 = \frac{(12\pi e\bar{\beta})^2}{q^6} (q_x q_y q_z)^2 == (12\pi e\bar{\beta})^2 \cos^4\theta \sin^2\theta \cos^2\varphi \sin^2\varphi. \tag{56}$$

Finally, the total probability of emission of phonon with a longitudinal polarization is given by the following expression:

$$W_{LPA} = \frac{18\hbar \left(e\bar{\beta}\right)^2 \varepsilon_{10}}{\rho\left(\hbar s\right)^3} \int d\theta \, d\varphi \left| I\left(\varepsilon_{10}\frac{\cos\theta}{\hbar s}, \varphi\right) \right|^2 \cos^4\theta \sin^2\theta \cos^2\varphi \sin^2\varphi \tag{57}$$

4.3.3 Emission of deformation acoustic phonon

The matrix element of interaction of an electron with a deformation field introduced in 1950 by J. Bardeen and W. Shockley [11] is given by

$$M_{DA} = \int d^3r \, \Phi'\left(\mathbf{r}\right)^* w\left(\mathbf{r}\right) \Phi\left(\mathbf{r}\right), \tag{58}$$

where value $w(r)$ is called deformation potential. The homogeneous deformation of crystal due to long-wave acoustic phonons is described by a tensor of deformation u_{ij}. Therefore in the lowest order on displacement of atoms deformation potential of acoustic phonons can be expand into a series of u_{ij} and to write down

$$w = \Xi^{ij} u_{ij} \tag{59}$$

(the summation on repeating indexes is performed). Values Ξ^{ij} (of the units of energy) are referred as constants of deformation potential. As the tensor u_{ij} is symmetrical, the same property has the tensor of constants of deformation potential Ξ^{ij}. The number of independent constants is determined by symmetry of Brillouin zone in that point $\mathbf{k}$, in which the influence of deformation on a spectrum is studied.

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The elementary case takes place in a cubic crystal, when the extremum of the band is located in a point $\mathbf{k} = 0$. The symmetrical tensor of the second rank in this case is reduced to one constant

$$\Xi^{ij} = \delta_{ij}\Xi. \tag{60}$$

Then

$$w = \Xi u, \qquad u = u_{11} + u_{22} + u_{33}, \tag{61}$$

where u - relative change of volume as a result of deformation. In this case deformation of shift which is not changing of volume, does not result in occurrence of deformation potential. From (24) and (25) one obtain

$$u_{ij}\left(\mathbf{r}, t\right)_{s\mathbf{q}} = \frac{1}{L^{3/2}} \left[\frac{\hbar a_0^3}{2M_0\omega_{s\mathbf{q}}}\right]^{1/2} \frac{1}{2}i\left(d_{s\mathbf{q}}^i q_j + d_{s\mathbf{q}}^j q_i\right) e^{i\mathbf{q}\mathbf{r}-i\omega_{s\mathbf{q}}t} + c.c. \tag{62}$$

Substituting (62) into (59), one find deformation potential from one acoustic phonon

$$w\left(\mathbf{r}, t\right)_{s\mathbf{q}} = \frac{1}{L^{3/2}} \left[\frac{\hbar a_0^3}{2M_0\omega_{s\mathbf{q}}}\right]^{1/2} e^{i\mathbf{q}\mathbf{r}-i\omega_{s\mathbf{q}}t}\Xi_{s\mathbf{q}}iq + c.c., \tag{63}$$

where the effective constant of deformation potential of wave is included

$$\Xi_{s\mathbf{q}} = \Xi^{ij}\frac{1}{2q}\left(d_{s\mathbf{q}}^i q_j + d_{s\mathbf{q}}^j q_i\right), \tag{64}$$

it depends only on a direction and polarization of phonon. In our case of cubic crystal we have $\Xi_{s\mathbf{q}} = \Xi$ (7 eV for GaAs for longitudinal phonons and $\Xi_{s\mathbf{q}} = 0$ for transverse ones [12]).

So, in Si and GaAs the deformation acoustic phonons only with a longitudinal polarization can be emitted. The matrix element will finally look like

$$M_{DA} = i\Xi\sqrt{\frac{\hbar}{2\rho s}}L^{-3/2}\sqrt{q}I\left(\mathbf{q}\right). \tag{65}$$

Then probability of deformation acoustic phonon $s\mathbf{q}$ emission

$$w_{10} = \frac{\pi\Xi^2}{\rho s L^3}q\left|I\left(\mathbf{q}\right)\right|^2 \delta\left(\varepsilon_{10} - \hbar sq\right). \tag{66}$$

Finally, substituting (66) into (30), passing to spherical coordinates by the rule (40) and making integration over delta-function, we have a total probability of generation of deformation acoustic phonon

$$W_{DA} = \frac{\Xi^2\varepsilon_{10}^3}{8\pi^2\hbar^4 s^5}\int_0^{2\pi}d\varphi\int_{-\pi/2}^{\pi/2}d\theta\cos\theta\left|I\left(\varepsilon_{10}\frac{\cos\theta}{\hbar s},\varphi\right)\right|^2 \tag{67}$$

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4.4   Results and discussion

The results of calculation of processes of decoherence by structure owing to spontaneous emission of particles are given in a Fig. 13. As it can be seen from the graphics the prevailing mechanism of decoherence is the emission of polarizing acoustic phonons. However, even this process has small probability at durations of step appropriate to a GHz range of clock frequencies for wide structures (wider than 15 nm). The energy splitting versus distance between electron density maxima r shown in Fig. 14 is far above temperature limit (5 mK). It is worth of noting, that the process of emission of polarizing acoustic phonons is characteristic for materials such as GaAs, in Si, for example, owing to symmetry of lattice they will not be generated. Thus, in Si the prevailing mechanism of decoherence will be emission of deformation acoustic phonons.

5   Conclusions

New quantum bit is offered on the basis of spatial states of electrons in symmetrical semi-conductor quantum dots controlled with the help of voltage on electrodes. The quantum-mechanical calculation of states of the offered qubit is fulfilled. The operation of the one-qubit gate which is carrying out unitary transformation, and not trivial two-qubit CNOT gate are simulated. The processes of decoherence were investigated. Our study comprises spontaneous emission of photon, deformation acoustic phonon and piezoelectric acoustic phonon. The work frequencies of the quantum register being built using offered quantum bits, lie in a range convenient for electronic control and achieve 1 GHz. The offered quantum register is scalable and its size is not limited. The structure reveals sufficient degree of coherence that allows by using of the appropriate methods of error correction to work during unlimited time. It is necessary to note, that offered quantum bit can be realized physically at an existing level of cryogenic engineering and nanoelectronic technology.
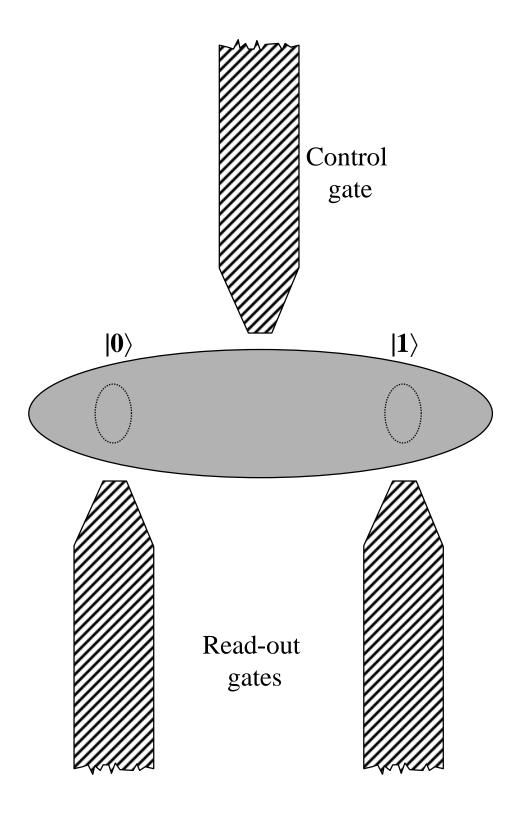
Acknowledgments

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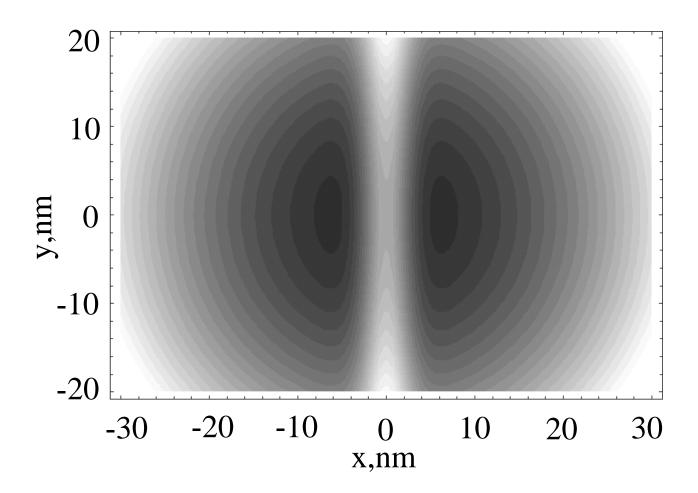
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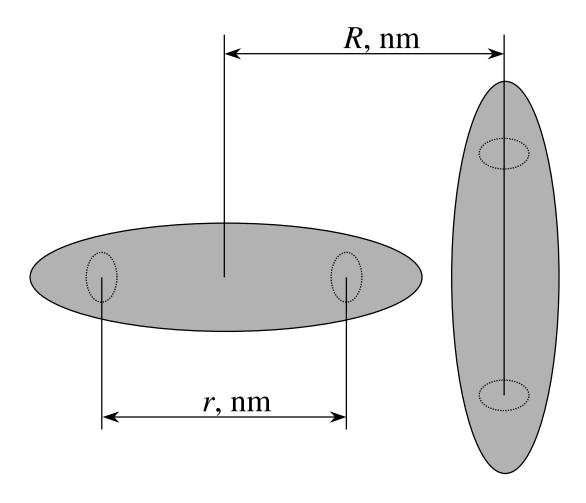
Figure captions

Fig. 1. Quantum dot qubit.

Fig. 2. Quantum dot potential profile (greyscale, whiter denotes the higher potential).

Fig. 3. Sketch of CNOT gate (r is a separation between electron density maxima; R is a separation between qubits' centers)

Fig. 4–7. Wavefunctions of four bottom states of an electron.

Fig. 8. Wavefunction of $|0\rangle$ qubit state.

Fig. 9. Wavefunction of $|1\rangle$ qubit state.

Fig. 10. NOT gate operation time diagram. V_g is a control gate voltage, $\Delta\omega$ is an energy separation between two bottom states.

Fig. 11. NOT gate duration versus distance between electron density maxima r.

Fig. 12. CNOT gate duration versus distance between dots centers R at different r.

Fig. 13. Decoherence due to spontaneous emission of photons and acoustic phonons versus r.

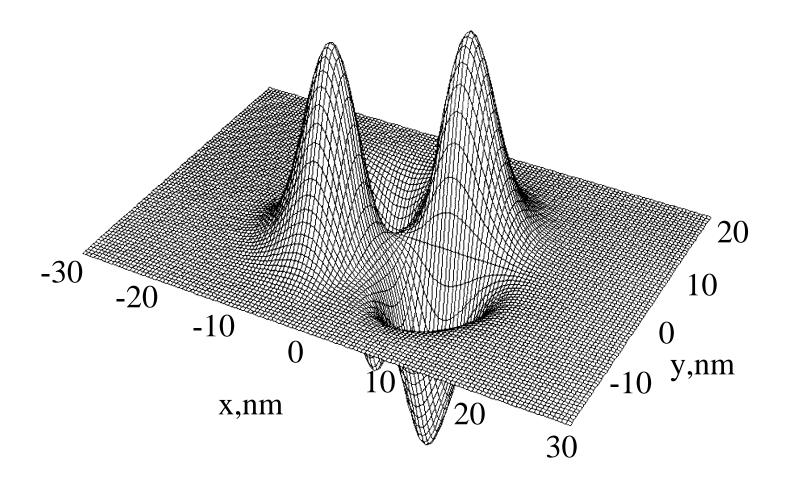Fig. 14. Energy splitting ε_{10} versus distance between electron density maxima r.

Control
gate

$|0\rangle$ $|1\rangle$

Read-out
gates

V(x,y)

Ψ_1

Ψ_2

Ψ_3

Ψ_4

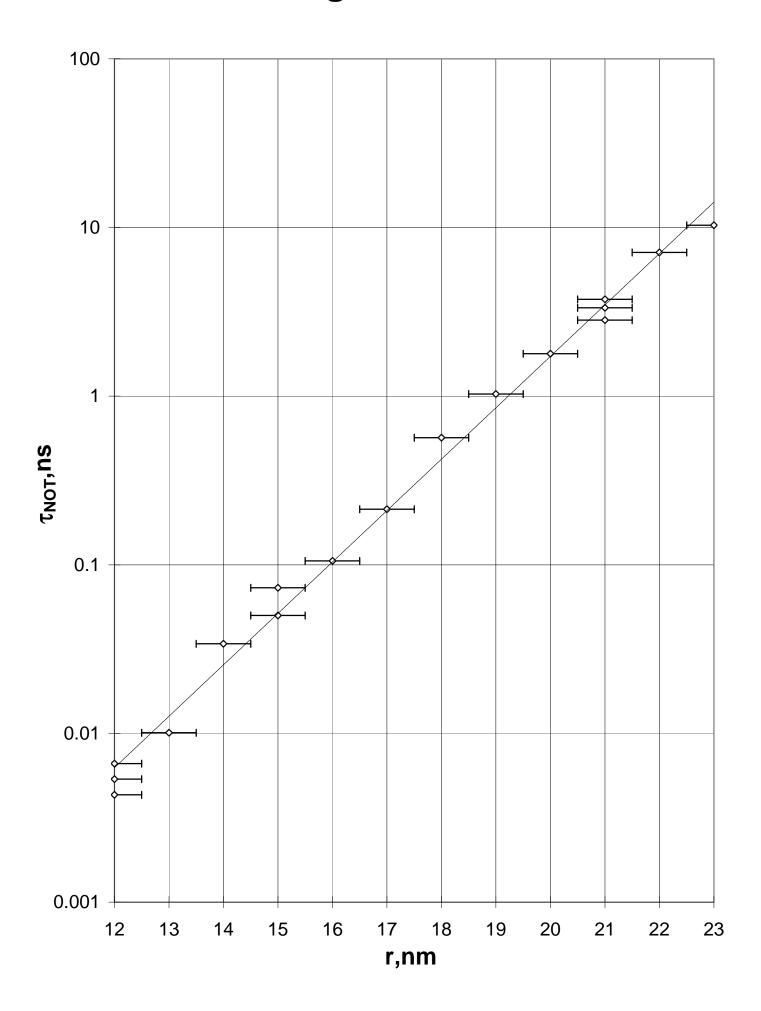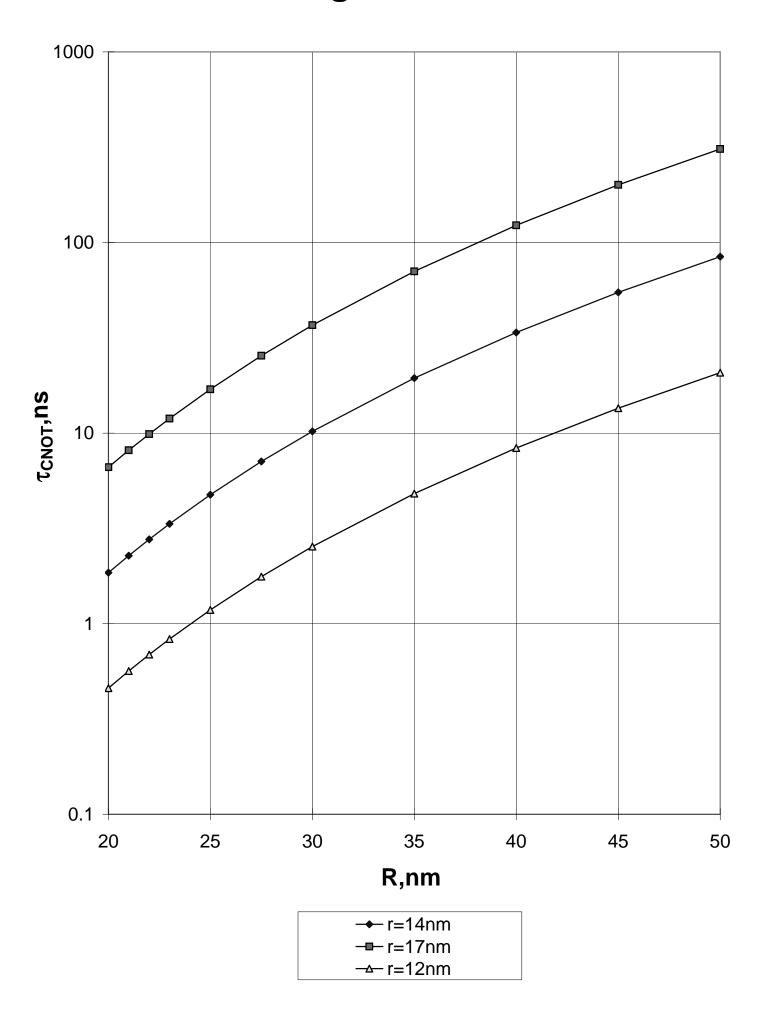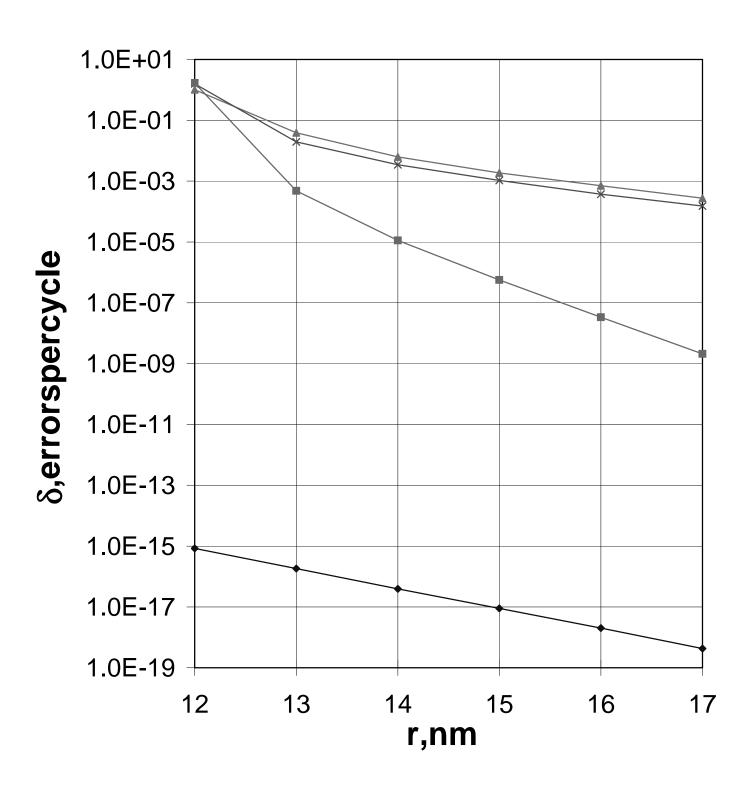$|0\rangle$
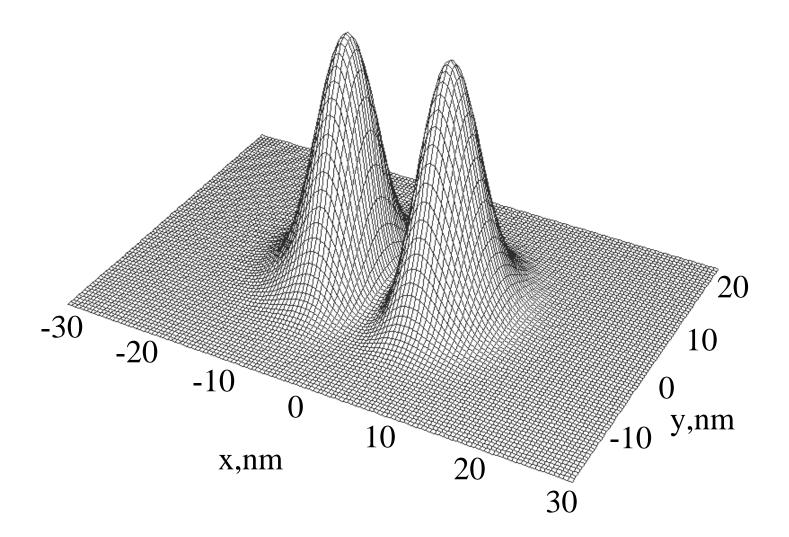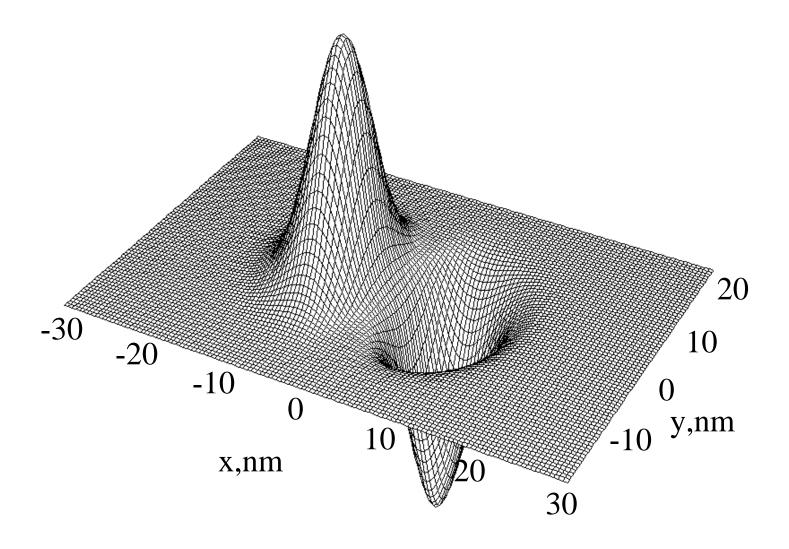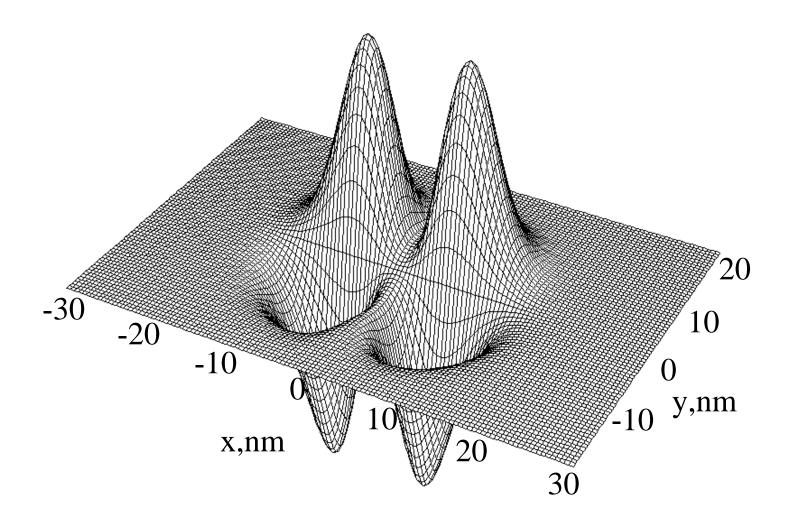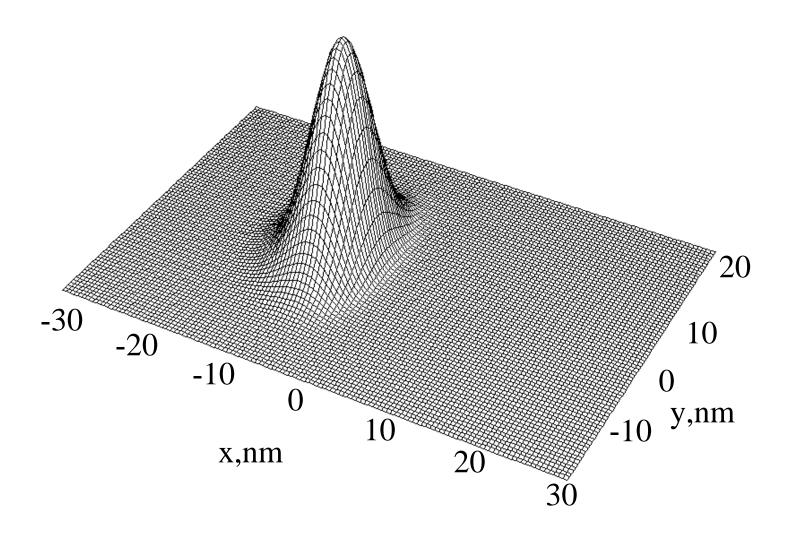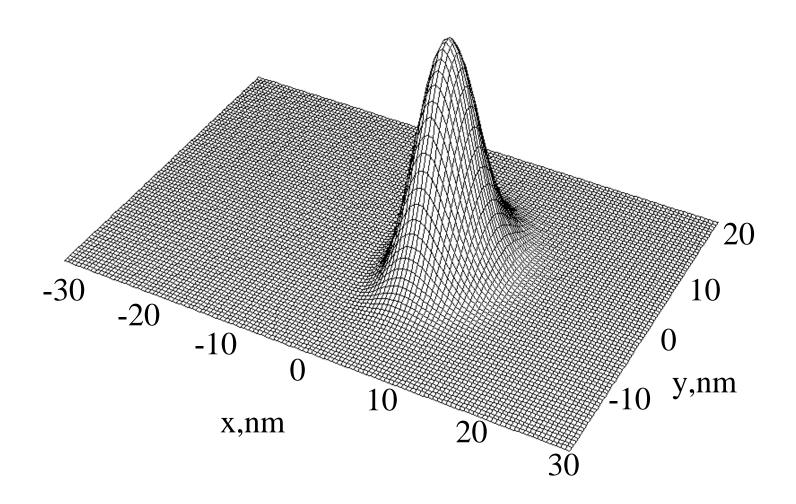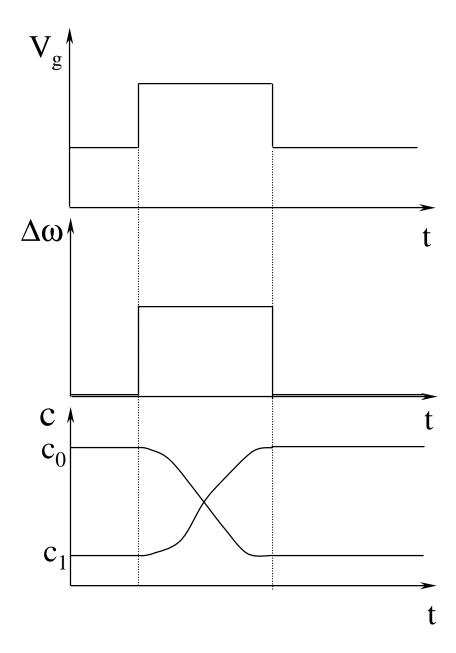
NOTgateduration

CNOTgateduration

Decoherence
(spontaneousemission)

Legend:
- photons(estimation)
- longitudinalpiezoelectricacousticphonons
- transversepiezoelectricacousticphonons
- deformationacousticphonons

Y-axis: δ,errorspercycle

X-axis: r,nm