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SINGLE-ELECTRON COMPUTING WITHOUT DISSIPATION

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A possibility to perform single-electron computing without dissipation in the array of tunnel-coupled quantum dots is studied theoretically, taking the spin gate NOT (inverter) as an example. It is shown that the logical operation can be realized at the stage of unitary evolution of electron subsystem, though complete switching of the inverter cannot be achieved in a reasonable time at realistic values of model parameters. An optimal input magnetic field is found as a function of inter-dot tunneling energy and intra-dot Coulomb repulsion energy.

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Recent advances in the fabrication of nanometer scale quantum dots open an opportunity of practical implementation of the idea to use the states of a quantum system for data coding and processing [1]. For example, the spins of individual electrons can be viewed as the bits of information: logical one (zero) corresponds to "up" ("down") direction of electron spin at a given quantum dot. *Spin gates* (elementary sets of quantum dots performing particular logical functions) have been discussed by Bandyopadhyay et al. [2] and later investigated theoretically by Molotkov and Nazin [3] and by Krasheninnikov and Openov [4]. If occupation/unoccupation of a quantum dot by a single electron is viewed as a bit 1/0, one has *charge gates*, various kinds of which have been studied, e.g., by Lent et al. [5] and by Nomoto et al. [6]. In arrays of quantum dots, the quantum tunneling of electrons between adjacent dots and/or Coulomb interaction of electrons with each other play a role of "wiring", resulting in the signal propagation from dot to dot.

The operation of spin and charge gates is based on the principle of "ground state computation" [2,5]. According to this principle, upon the influence of external source on input dots of a particular gate, the electron subsystem changes to a new ground state. The final spin or charge configuration reflects the result of "calculation". This result can be read from output dots of the gate. The quantum dot gates are believed to possess high-speed performance as a consequence of extremely fast switching between different electron ground states. However, the switching rate, being dictated by dissipation processes, is not known *a priori*. For a gate consisting of a few quantum dots and operating at sufficiently low temperatures, the switching rate may appear to be rather small (10^6 to 10^9 s^{-1} [6]), thus slowing down the computation. Hence, in studies of the potential of quantum dot arrays for high-speed single-electron computing one should give special attention to inelastic relaxation processes.

An alternative way has been discussed recently by Bandyopadhyay and Roychowdhury [7]. They explored the dynamic behavior of the simplest spin gate NOT (inverter) and found that there exists optimal input signal energy to achieve its *complete* switching in the absence of inelastic relaxation. However, it remains

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unclear how adequately the results obtained in [7] depict reality since the authors of Ref.[7] used the Heisenberg model to describe the correlated electrons in quantum dots. Meanwhile, it is well known that this model is just a limiting case of more realistic Hubbard model [8] and cannot be used if the inter-dot electron tunneling energy V is of the order or greater than the intra-dot electron repulsion energy U. It is instructive to study the broad range of V and U values in order to see if the conclusions of [7] reflect the basic physics or are just a consequence of using a particular theoretical model.

In this paper we study the unitary evolution of electron subsystem in the spin gate NOT (inverter) making use of the Hubbard model with arbitrary values of V and U. The inverter consists of two closely spaced quantum dots (A and B) occupied by two electrons [2, 3, 7]. One of two dots (say, the dot A) serves for writing the input signal to the gate by the action of the local magnetic field H_A. The second dot (B) is the output. At $H_A = 0$ the ground state of the inverter is the entangled state with zero magnetic moments at both dots A and B. The logical function NOT is realized if at $H_A \neq 0$ magnetizations (i.e., spin projections) of dots A and B have opposite directions. *Complete* switching of the inverter is said to take place if spin projections are saturated ($S_{zA} = 1/2$, $S_{zB} = -1/2$ or $S_{zB} = 1/2$, $S_{zA} = -1/2$, where $S_{zi} = \langle \hat{S}_{zi} \rangle = \langle \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} \rangle /2$, $\hat{n}_i$ being the operators of particles number at dots $i = A, B$). Upon complete switching, magnetizations of both dots reach the maximum absolute value $g\mu_B$, where g is the Lande factor, μ_B is the Bohr magneton. We stress that the ground state at any *finite* value of H_A is organized in such a way that $|S_{zA}| < 1/2$ and $|S_{zB}| < 1/2$ [3, 7]. Hence, the complete switching of the inverter cannot be achieved through its *inelastic relaxation* to a new ground state.

The Hubbard Hamiltonian for the inverter has the form

$$\hat{H} = -V \sum_{\sigma} (\hat{a}^{+}_{A\sigma} \hat{a}_{B\sigma} + \hat{a}^{+}_{B\sigma} \hat{a}_{A\sigma}) + U \hat{n}_{A\uparrow} \hat{n}_{A\downarrow} + U \hat{n}_{B\uparrow} \hat{n}_{B\downarrow} - g\mu_B H_A \sum_{\sigma} \hat{n}_{A\sigma} \mathrm{sign}(\sigma), \quad (1)$$

where the quantities V, U, H_A, g, and μ_B are defined above, other notations being standard (see, e.g., [4]). Here we assume that each dot has one size-quantized level with on-site potential $\varepsilon_0 = 0$ (i.e., all energies are measured from ε_0). In what follows, we set $g\mu_B = 1$.

The complete orthonormal set of inverter eigenstates is formed by two-electron basis states $|1\rangle = |\uparrow, \downarrow\rangle$, $|2\rangle = |\downarrow, \uparrow\rangle$, $|3\rangle = |\uparrow\downarrow, 0\rangle$, $|4\rangle = |0, \uparrow\downarrow\rangle$, $|5\rangle = |\uparrow, \uparrow\rangle$, $|6\rangle = |\downarrow, \downarrow\rangle$, where, e.g., the notation $|\uparrow, \downarrow\rangle$ denotes the state with up-spin electron at the dot A and down-spin electron at the dot B, the notation $|\uparrow\downarrow, 0\rangle$ denotes the state with two (up-spin and down-spin) electrons at the dot A and no electrons at the dot B, etc. The magnetic moment of the electron with up-spin polarization is oriented along the direction of the local applied magnetic field H_A.

At $H_A = 0$, the ground state eigenvector of the Hamiltonian (1) is

$$\Psi_0 = \frac{1}{2} \sqrt{1 + \frac{U}{\sqrt{U^2 + 16V^2}}} \left(|1\rangle + |2\rangle + \frac{\sqrt{U^2 + 16V^2} - U}{4V} |3\rangle + \right.$$

$$\left. + \frac{\sqrt{U^2 + 16V^2} - U}{4V} |4\rangle \right). \quad (2)$$

The corresponding eigenenergy is $E_0 = (U - \sqrt{U^2 + 16V^2})/2$. In the ground state we have $\langle\Psi_0|\hat{S}_{zA}|\Psi_0\rangle = \langle\Psi_0|\hat{S}_{zB}|\Psi_0\rangle = 0$. We suppose that at $t \leq 0$ the system is in its ground state.

If the local external magnetic field is applied at time $t = 0$, then the wave function $\Psi(t)$ at $t \geq 0$ is

$$\Psi(t) = \sum_{k=1}^{6} A_k \Psi_k \exp(-iE_k t/\hbar), \tag{3}$$

where Ψ_k and E_k $(k = 1 - 6)$ are eigenvectors and eigenenergies of the stationary Schrödinger equation

$$\hat{H}\Psi_k = E_k \Psi_k. \tag{4}$$

The coefficients A_k should be found from the initial condition $\Psi(t = 0) = \Psi_0$. It is convenient to write Ψ_k as

$$\Psi_k = \sum_{n=1}^{6} B_{kn}|n\rangle. \tag{5}$$

Then

$$\Psi(t) = \sum_{n=1}^{6} f_n(t)|n\rangle, \tag{6}$$

where

$$f_n(t) = \sum_{k=1}^{6} A_k B_{kn} \exp(-iE_k t/\hbar). \tag{7}$$

The probability to find the system in the basis state $|n\rangle$ at time t is $p_n(t) = |f_n(t)|^2$.

At arbitrary values of V, U, and H_A the eigenvalue equation (4) reduces to the algebraic equation of the third power in E_k. The resulting analytic expressions are too cumbersome for analysis, so it is more convenient to solve the equation (4) numerically. Before proceeding to the results of these calculations, let us consider the limiting case $U = 0$ which physically corresponds to $U << V$ (closely-spaced large-sized dots [6]).

At $U = 0$ we have rather simple equations for the probabilities $p_n(t)$:

$$p_1(t) = \frac{1}{4}\left(1 + \frac{4H_A V}{H^2 + 4V^2}\sin^2(\omega t/2)\right)^2, \quad p_2(t) = \frac{1}{4}\left(1 - \frac{4H_A V}{H^2 + 4V^2}\sin^2(\omega t/2)\right)^2,$$

$$p_3(t) = p_4(t) = \frac{1}{4}\left(1 - \frac{16H_A^2 V^2}{(H^2 + 4V^2)^2}\sin^4(\omega t/2)\right), \quad p_5(t) = p_6(t) = 0, \tag{8}$$

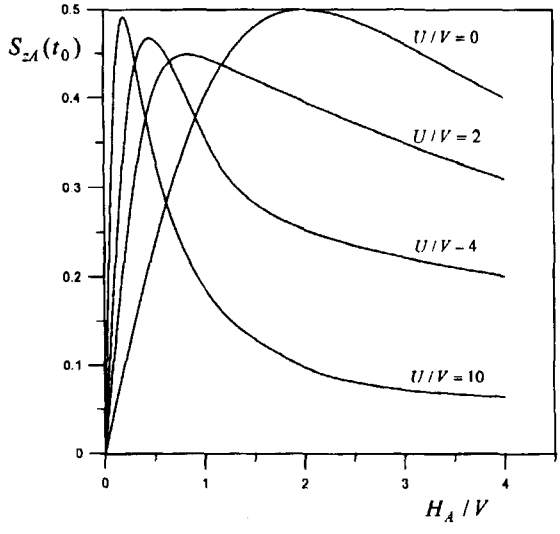
where $\omega = \sqrt{H_A^2 + 4V^2}/\hbar$. From (6) and (8) it is straightforward to find that

$$S_{zA}(t) = \langle\Psi(t)|\hat{S}_{zA}|\Psi(t)\rangle = -S_{zB}(t) = (p_1(t) - p_2(t))/2 = \frac{2H_A V}{H_A^2 + 4V^2}\sin^2(\omega t/2). \tag{9}$$

From (9) we see that the spins S_{zA} and S_{zB} are oppositely directed at any time t according to the physical truth table of the logical gate NOT [3]. For the sake of definiteness, let us consider the case $H_A > 0$. In this case S_{zA} is always positive and peaks at $t_0 = \pi/\omega$. Moreover, a *complete* switching, $S_{zA}(t_0) = 1/2$ and $S_{zB}(t_0) = -1/2$, is achieved at $H_A/V = 2$. The dependence of $S_{zA}(t_0)$ on H_A/V

is shown in Figure. We stress that this dependence has been obtained by us in the weak coupling limit of the Hubbard model. Nevertheless, it is analogous to those calculated in [7] within the Heisenberg model (i.e., in the strong coupling limit of the Hubbard model, $U >> V$) with an exception that in the Heisenberg model $\omega = \sqrt{H_A^2 + 4J^2}/\hbar$, $t_0 = \pi/2\omega$, and $S_{zA}(t_0)$ reaches a maximum value of $1/2$ at $H_A = 2J$ [7], where J is the antiferromagnetic exchange energy (for two-site cluster $J = V^2/U$ at $U >> V$). Hence, one may expect that complete switching of the inverter can occur at an *arbitrary* ratio of U to V.

To check this hypothesis, we calculated numerically the dependencies of S_{zA} on t and $S_{zA}(t_0)$ on H_A/V at different values of U/V, where t_0 is generally defined as a time of the first maximum at the curve $S_{zA}(t)$, t_0 being a function of H_A/V and U/V. The curves of $S_{zA}(t_0)$ versus H_A/V are shown in Figure for several values of U/V. One can see that increase in U/V first results in decreased height of the maximum at the $S_{zA}(t_0)$ versus H_A/V curve. At $U/V > 2$ the height of this maximum increases again, but doesn't reach the saturated value $1/2$ at finite U/V, though $S_{zA}(t_0) \to 1/2$ if $U/V \to \infty$ (this corresponds to the Heisenberg model and agrees with the results obtained in [7]).



The maximum value of $S_{zA}(t_0)$ versus H_A/V at different U/V

It seems that complete switching of the inverter cannot be achieved at realistic values of U/V ratio, i.e., at $U/V \neq 0$ and $U/V \neq \infty$. Note, however, that at arbitrary values of H_A/V and U/V the function $S_{zA}(t)$ is not periodic in time since it includes several harmonics with different frequencies and amplitudes. Hence, in principle, the value of $S_{zA} = 1/2$ can be achieved at some longer time. But this case is of no interest for us since we should like not only to reach the maximum permissible value of S_{zA}, but to do it in as short as possible switching time.

However, an impossibility to achieve the complete switching of the inverter doesn't imply the impossibility to perform the logical operation NOT at the stage of the unitary evolution. One should just to "read" the signal at a time when $S_{zA(B)}$ has a large absolute value, e.g., at a time t_0. Indeed, $S_{zA}(t_0) \geq 0.45$ at any value of U/V (see Figure). Hence, the error probability $P_{err} = 1 - p_1(t_0)$ (i.e., the probability to read the "wrong" signal $S_{zA} = -1/2$ or $S_{zA} = 0$ at a time t_0) is

less than 0.1. Our calculations showed that at $U/V << 1$ and at 'optimal' (for a given U/V) value of H_A/V the time t_0 is of the order of $\hbar/V$, i.e., $t_0 \approx 10^{-13}s$ for $V \approx 10$ meV. The value of t_0 increases as U increases and reaches $\approx 6\hbar/V$ at $U/V = 10$. The limiting value of t_0 at $U >> V$ is $t_0 = \pi\hbar U/4\sqrt{2}V^2$, in accordance with [7]. Thus, to speed up the calculation, we should have small U and large V. If the shape of a single quantum dot is a cube with side length a and the distance between the quantum dots is d, then V decreases exponentially in both d and a, while U is roughly inverse proportional to a and is almost independent on d [6, 9]. Hence, small values of d and a favor short switching times t_0 (the values of U and V can be calculated numerically for a given set of geometrical parameters of quantum dots array and for a particular choice of semiconducting materials [6]).

On the other hand, the 'optimal' value of H_A increases with V as $H_A^{opt} = 2V$ at $U = 0$ (9) and as $H_A^{opt} = 2V^2/U$ at $U/V >> 1$ (see also [7]). The product $H_A^{opt}t_0$ is of the order of $\hbar$ at any U/V. Hence, one can have a realistic value of $H_A^{opt} < 1$ Tesla only at the expense of increasing t_0 up to $\approx 10^{-11}$s. Nevertheless, this value of t_0 still remains several orders of magnitude smaller than characteristic times of inelastic relaxation [6].

In summary, the switching of the spin gate NOT (inverter) at the stage of unitary evolution is much faster than through relaxation to a new ground state. The switching time can be reduced down to 10^{-11}s through proper choice of quantum dots geometrical parameters and local external magnetic field, with the error probability less than 0.1.

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