Pis'ma v ZhETF, vol.64, iss.3, pp.214 - 218 © 1996 August 10

ELEMENTARY QUANTUM DOT GATES FOR SINGLE-ELECTRON COMPUTING

A.V.Krasheninnikov, L.A.Openov

Moscow State Engineering Physics Institute[1]

115409 Moscow, Russia

Submitted 4 July 1996

A new approach to realization of particular logical functions in quantum dot gates for single-electron computing is proposed. It is shown that placing a gate into a uniform external magnetic field allows one to construct gates with 1) symmetric physical truth tables and 2) large (in some cases close to saturated) absolute magnitude of the average spin at output dots. Thus, two serious obstacles are removed which otherwise could present a problem in fabrication of a set of coupled quantum dot gates.

PACS: 73.20.Dx, 84.30.Bv, 85.30.Vw

In recent few years an idea of constructing the so called quantum computer [1−4] as well as a computer [5−7] based on quantum effects but employing classical Boolen logic has been discussed in the literature [1−7]. Such computers are thought to be composed of coupled elementary gates. Each gate realizes a particular logical function (e.g., NOT, AND, OR, etc.). One way to perform calculations is based on idea of ground state computing, when the result of a logical operation always corresponds to the ground state of the gate. Upon changing the ground state through an external influence, one has a new ground state which contains information on the results of calculations.

In this paper we restrict ourselves to quantum dot gates (spin gates) [5-7]. Such gates consist of a number of quantum dots at a solid surface. Each dot is supposed to have a single energy level and there is, on the average, one electron per dot. The tunneling of electrons between dots plays a role of quantum wires. In such a system, the bits of information are carried by spins of individual electrons: the logical unit (zero) corresponds to the "up" ("down") direction of electron spin at a given dot.

Each gate has input and output dots. The former serve for writing the input signals to the gate (e.g., by making use of local magnetic field generated by a magnetic tip of STM). After the action of external influence on input dots, the spin configuration of the gate changes as a result of subsequent spin switching on adjacent dots due to electron-electron interactions. The new ground state represents the result of calculations which can be read from output dots by means of, e.g., magnetic tip (keeping in mind that the tunneling current depends on the mutual orientation of the dot and tip magnetizations). The correspondence between magnetizations of output and input dots is uniquely determined by the logical truth table of a particular gate. For example, the logical truth tables of NOT-AND and NOT-OR gates are shown in Fig.1.

Recently Molotkov and Nazin [6] have shown that there are no fundamental limitations on the physical realization of elementary spin gates and that for any

[1] e-mail: arc@supercon.mephi.ru

Not-AND Gate		
A	B	Y
1	1	0
0	1	1
1	0	1
0	0	1

Not-OR Gate		
A	B	Y
1	1	0
0	1	0
1	0	0
0	0	1

Fig.1. Logical truth tables of NOT-AND, and NOT-OR gates. A and B are the inputs; Y is the output

gate it is in fact possible to find the range of system parameters where the entire truth table is realized. This can be done in the presence of intradot Coulomb repulsion only, without direct exchange interaction of electrons on neighboring dots [6]. The relevant Hubbard-like Hamiltonian has the form:

$$H = -t \sum_{<ij>,\sigma} (a^+_{i\sigma} a_{j\sigma} + H.c.) - \mu_B \sum_{i,\sigma} n_{i\sigma} H_i \mathrm{sign}\sigma + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $a_{i\sigma}$ ($a^+_{i\sigma}$) is the operator of annihilation (creation) of electron on the i-th dot with spin projection σ = +1 or -1 on the z-axis, $n_{i\sigma} = a^+_{i\sigma} a_{i\sigma}$ is the electron number operator, t is the matrix element for hopping of electrons between quantum dots, U is the intradot Coulomb repulsion energy, H_i is the local magnetic field (along z-axis) at the i-th dot, μ_B is the Bohr magneton, $<ij>$ means the summation over nearest neighbor dots.

At half-filling ($\sum_{i,\sigma} n_{i\sigma} = N_{tot}$, where N_{tot} is the total number of dots in the gate) and at large enough ratio of U/t, there are strong antiferromagnetic interactions in the gate. These interactions result in the switching of electron spins throughout the gate after the action of local fields H_i on the input dots. The relevant "antiferromagnetic" physical realization of the NOT-AND gate is shown in Fig.2a.

To find the resulting values of electron spin at input and output dots after the action of local fields, one should know the ground state wave function of the Hamiltonian (1). In the case of relatively small (<12) number of dots in the gate, this can be done numerically by means of exact diagonalization method [8]. Doing so, one can find the physical truth table [6,7], i.e., the range of control signals (local magnetic fields at the input dots) in which the logical truth table of a particular gate is realized.

Since in a real system the electron spin at any quantum dot is never directed strictly "up" or "down", it is convenient to introduce the threshold value S_t (0 < S_t < 1) of the projection of electron spin on the axis z, so that the cases $\langle S_{iz}\rangle > S_t/2$ and $\langle S_{iz}\rangle < -S_t/2$ correspond to logical unit and zero respectively [7]. Here i is the number of a particular quantum dot in the gate, $\langle S_{iz}\rangle = \langle (n_{i\uparrow} - n_{i\downarrow})\rangle$.

To understand how the physical truth table for a particular gate can be constructed, let us consider the NOT-AND gate (Fig.2a). The values of $\langle S_A\rangle$, $\langle S_B\rangle$, and $\langle S_Y\rangle$, are calculated by means of exact diagonalization [8] of Hamiltonian (1) at many different values of H_A and H_B. If, e.g., $\langle S_A\rangle > S_t/2$, $\langle S_B\rangle > S_t/2$, and $\langle S_Y\rangle < -S_t/2$ at given values of H_A and H_B, then the first row (110) of the logical truth table of the NOT-AND gate (see Fig.1) is realized, and we

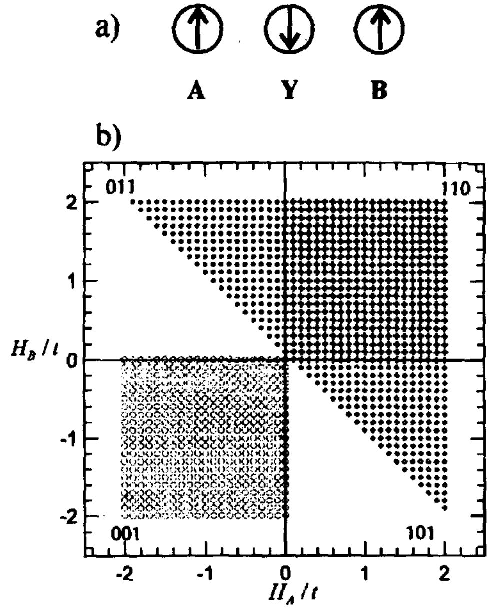

Fig.2. Three-dot NOT-AND gate. *a*) physical realization; *b*) physical truth table for $U/t = 20$; $S_t = 0.05$; H_A and $H_B Z$ are local magnetic fields at A and B dots respectively

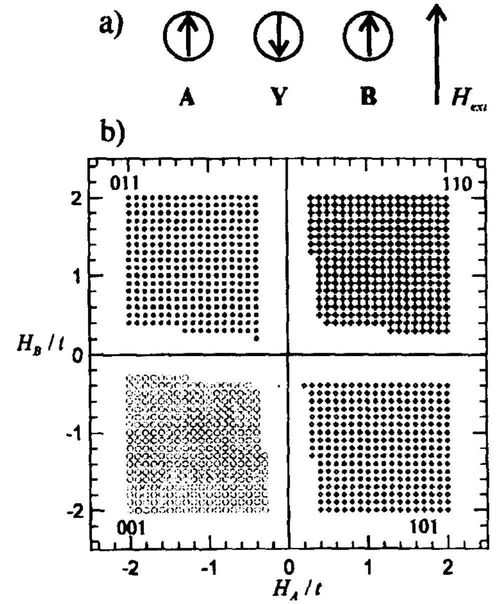

Fig.3. The same as in Fig.2, but $S_t = 0.95$ and the uniform external magnetic field with $\mu_B \cdot H_{oz} = 0.01t$ is applied to the whole gate

mark the point (H_A, H_B) in the $H_A - H_B$ plane by the symbol "+". If the spin configuration corresponds to one of the other three rows of the logical truth table (011, 101, or 001), then the point (H_A, H_B) is also marked by the corresponding symbol. The blank space in the $H_A - H_B$ plane means that none of the rows of the logical truth table is realized at given values of H_A and H_B.

We stress that the value of S_t should not be too small in order one could discriminate unambiguously between configurations with spin up and spin down, i.e., between logical unit and logical zero. However, it turned out [6,7] that for all gates considered, except the simplest two-dot NOT gate, the magnitude of the average spin $\langle S_{iz} \rangle$ at the output is rather small. Moreover, physical truth tables are asymmetric with respect to input signals [6,7].

The calculated physical truth table of the NOT-AND gate is shown in Fig.2*b* for the case $S_t = 0.05$ (see also Fig.4 in [6]). One can see that even for S_t as low as 0.05, the 011 and 101 rows of the logical truth table (Fig.1) are never realised at *equal* absolute values of H_A and H_B (the situation becomes significantly worse as S_t increases). This fact has detrimental effect if one wishes to integrate the gate into the computational network [7].

In this paper we suggest a new approach to constructing spin gates and remove the two obstacles mentioned above (small values of S_t and asymmetry of physical truth tables). First, we illustrate our idea taking the NOT-AND gate as an example. We note that the apparent reason for the asymmetry of the physical truth table of the NOT-AND gate (Fig.2*b*) is that the rows 011 and 101 of the logical truth table (Fig.1) are unfavorable from the point of view of

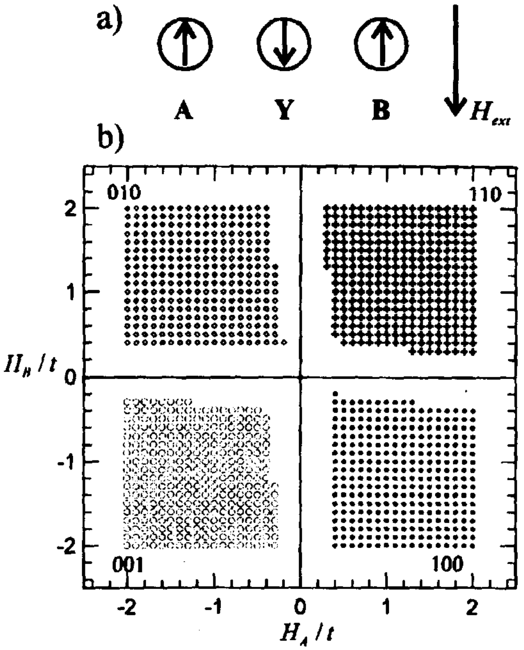

Fig.4. Three-dot NOT-OR gate. *a)* physical realization; *b)* physical truth table for $U/t = 20$; $S_t = 0.95$. The uniform external magnetic field with $\mu_B \cdot H_{oz} = -0.01t$ is applied to the whole gate

"antiferromagnetic ideology". Indeed, if the local fields at input (edge) dots A and B are equal in magnitude but different in sign, $H_A = -H_B$, then electron spins at dots A and B have opposite directions, while $\langle S_Y \rangle = 0$ at the output (central) dot Y since the electron spin at Y is frustrated. It means that two ground-state spin configurations, e.g., $\downarrow\uparrow\uparrow$ and $\downarrow\downarrow\uparrow$ spin arrangements at dots AYB are degenerate in the case $H_A < 0$ and $H_B > 0$.

Note, however, that the row 011 of the NOT-AND's logical truth table can be realized if the spin configuration $\downarrow\uparrow\uparrow$ corresponds to the nondegenerate ground state. This can be achieved easily by applying a uniform magnetic field with $H_{oz} > 0$ to the whole gate and thus removing the degeneracy of $\downarrow\uparrow\uparrow$ and $\downarrow\downarrow\uparrow$ spin configurations in favour of the former one. We stress that the value of H_{oz} should not be too large; otherwise unwanted configuration $\uparrow\uparrow\uparrow$ can occur even in the case $H_A < 0$. In other words, the value of $\mu_B H_{oz}$ should be less than the difference between the energies of $\uparrow\uparrow\uparrow$ and $\downarrow\uparrow\uparrow$ configurations. Since the latter is of the order of the hopping matrix element, t, the inequality

$$\mu_B |H_{oz}| \ll t \tag{2}$$

is sufficient for $\downarrow\uparrow\uparrow$ to be the ground state spin configuration. The same is true for the $\uparrow\uparrow\downarrow$ configuration that corresponds to the row 101 of the logical truth table.

The calculated physical truth table of the NOT-AND gate in the uniform external magnetic field with $\mu_B H_{oz} = 0.01t$ is shown in Fig.3. One can see that the case $H_{oz} > 0$ offers two important advantages over the case $H_{oz} = 0$ (see Fig.2). First, note that the threshold value $S_t = 0.95$ is very close to unity, i.e., external magnetic field results in almost saturated average spins at both input and output dots. Obviously, it is much more easier to read the information from the output dot with a large magnetic moment at it (we recall that the results presented in Fig.2 are for $S_t = 0.05 \ll 1$).

Second, at $H_{oz} > 0$ the physical truth table is symmetrical in the sense that domains corresponding to different rows of the logical truth table are located around diagonals ($H_A = \pm H_B$), and, moreover, occupy almost all floor space in the $H_A - H_B$ plane. As noted in [7], this is the most suitable situation for integration the gate into the computational network in which output dots of one gate serve as input dots of the other gates, and vice versa.

We proceed with the NOT-OR gate. It is seen from Fig.1 that the logical truth tables of NOT-OR and NOT-AND gates differ only in their second and third rows. We recall that in the NOT-AND gate these are the rows that correspond to "dangerous" spin configurations $\downarrow\uparrow\uparrow$ and $\uparrow\uparrow\downarrow$, while in the NOT-OR gate the configurations $\downarrow\downarrow\uparrow$ and $\uparrow\downarrow\downarrow$ should be realized. One can see that the latter two configurations can be stabilized in same way as in the case of the NOT-AND gate, i.e., by applying a uniform magnetic field to the whole three-dot gate. The difference is just that magnetic field should be directed in the opposite direction as compared with the NOT-AND gate, i.e., $H_{oz} < 0$. The inequality (2) must be fulfilled as well.

The calculated physical truth table of the NOT-OR gate in the uniform external magnetic field with $\mu_B H_{oz} = -0.01t$ is shown in Fig.4. Here again, as in the case of the NOT-AND gate (Fig.3), the threshold value $S_t = 0.95$ is close to unity, and the physical truth table is symmetrical and consists of domains occupying almost all floor space in the $H_A - H_B$ plane. We stress that both NOT-AND and NOT-OR gates can be employed on the basis of the same three-dot physical realization, the difference being only in the direction of the external magnetic field. This is very important from the experimental point of view.

To conclude, we have shown that NOT-AND and NOT-OR quantum dot gates with symmetrical physical truth tables and almost saturated average spins at input and output dots can be realized on the basis of three-dot structure by applying a properly directed external magnetic field to the whole gate. Such gates can be readily integrated into the computational network and together with the simplest NOT gate (invertor) can be used for realization of other logical operations (AND, OR, XOR, ADDER, etc.) needed to perform calculations.

This work was supported by the Russian Foundation for Fundamental Research under Grant No 96-02-18918. A.V. Krasheninikov acknowledges the financial support from Samsung Electronics. We are grateful to S. N. Molotkov and S. S. Nazin for supplying us with preprints of their papers prior to publication and for many valuable comments. We thank V. F. Elesin and E. G. Kholmovskii for helpful discussions.

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