Single-electron spin logical gates

S. N. Molotkov and S. S. Nazin
Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow District, 142432 Russia

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The possibility of implementing the simplest logical operations on the basis of single-electron spin gates, in which information is coded by single electron spins, is considered. It is shown that there are no fundamental limitations to the physical realization of such gates (it is possible to find a range of system parameters in which the entire truth table can be realized). However, for some types of the gates the magnitude of the average spin (which carries the information) proves to be rather small, which can present a serious problem for attempts at real fabrication of these gates. © *1995 American Institute of Physics.*

The ideas of using the states of a complex quantum mechanical system for information coding were put forward rather long ago. The first serious analysis of the feasibility of calculations with the quantum computer appears to have been undertaken by Feynman.[1] After that, various physical systems were suggested for the physical realization of quantum logical gates.[2–6] A quantum computer is a set of elementary logical gates. Depending on the external influence (control signals acting on the inputs of one or several gates), interacting parts of a complex quantum mechanical system change their states implementing the required logical operation. Systems whose parts are coupled to each other by the electron–electron interaction rather than classical interconnections (e.g., wiring) have been given a special name "quantum coupled architecture." The second basic idea is "ground state computing," which means that the result of a particular logical operation corresponds to the ground state wave function of the system. An external influence changes the ground state of the system so that the final ground state represents the result of the calculations.

Recent advances in scanning tunneling microscopy (STM) open the way for fabrication of logical gates at the level of single molecules. STM allows one to manipulate single atoms at the surface[7] to detect single electron spins at both nonmagnetic[8] and magnetic surfaces,[9,10] and to produce atomic-scale quantum dots.[11]

One of the systems suitable for the realization of quantum spin gates is a set of tunnel-coupled quantum dots at the surface. We shall consider spin gates[12] in which information is coded by single electron spins. These gates can be realized if the following conditions are satisfied:

1) antiferromagnetic ordering: either intradot Coulomb repulsion or an interdot antiferromagnetic exchange interaction between electrons should take place (actually, the exchange interaction can be ferromagnetic, although in that case the Coulomb repulsion must be sufficiently large);

2) the geometry of the dot system layout at the surface should be chosen in such a

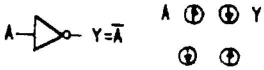


FIG. 1. Spin invertor.

way that only the nearest-neighbor interaction between the dots is important;

3) the average number of electrons in the system should be equal to the number of dots in the gate.

The external influence on the inputs (quantum dots) is realized by a local magnetic field which in principle can be produced using a magnetic tip similar to those used in atomic-force microscopy (AFM). Observations of single spins[8] and magnetic ions at the surface[10] with atomic resolution (~5 Å) represent a promising advance.

The "reading" and "writing" mechanism at the gate input and output consists in the local action of the tip magnetic field (in the absence of any current between the tip and the dot, similar to AFM) and subsequent spin switching in the adjacent quantum dots due to the electron–electron interactions in the system. Our aim is to determine the ranges of the system parameters and magnetic fields corresponding to the ground state wave function (actually, we are interested in the quantum-mechanical average spin at the quantum dots) representing the required line in the truth table of the specified logical function. It is not obvious whether there exists a set of system parameters that will permit one to realize the entire truth table by varying the "input" magnetic fields only.

We shall first consider qualitatively some simple logical gates.[12] The simplest gate is the invertor, which has one input (A) and one output (Y). Its truth table has the following form:

A	Y
1	0
0	1

Logical one (zero) corresponds to the spin "up" ("down") direction. The physical system implementing such a gate consists of two quantum dots with an antiferromagnetic interaction between them (Fig. 1).

In a simple picture, if the magnetic field at input A forces the spin upwards, the interaction keeps the electron spin at the output Y downwards and vice versa. However, the problem actually requires a consistent quantum-mechanical treatment which will be presented below.

The next in complexity is the NOT-AND (NAND) gate, which has two inputs (A and B) and one output (Y). The truth table can be written in the following form:

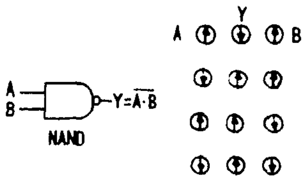


FIG. 2. The spin gate realizing the logical NOT-AND function.

A	Y	B
1	0	1
0	1	1
1	1	0
0	1	0

The corresponding physical system consists of three quantum dots, inputs A and B being driven by the local magnetic fields (Fig. 2).

The first line in the truth table is realized rather easily. If the local magnetic fields at inputs A and B force the spin upwards, the antiferromagnetic interaction keeps the spin at output Y downwards. Local magnetic fields lift the degeneracy between the $\uparrow\downarrow\uparrow$ and $\downarrow\uparrow\downarrow$ states. Hence, the one can realize in this way the first line in the truth table (actually the problem turns out to be more difficult). At first glance, it is not obvious whether or not the second and third lines in the truth table can be realized; nevertheless, we shall show that the answer is positive.

The next in complexity is the logical AND gate, which is obtained by adding the inverted output to the preceding NAND gate, resulting in the following truth table:

A	Y	B
1	1	1
0	0	1
1	0	0
0	0	0

It is realized by a system consisting of four quantum dots (Fig. 3).

The exchange interaction should keep the outputs Y and $\bar{Y}$ in the opposite states. By adding consecutively new quantum dots one can construct any gate (triggers, adders, etc.).[12]

Now we shall consider the problem in more detail. To describe a set of quantum dots we use a Hubbard-like Hamiltonian which also includes the exchange interaction between adjacent dots (similar to the Heitler–London approach[13]), assuming that there is only one size-quantized level in each quantum dot:

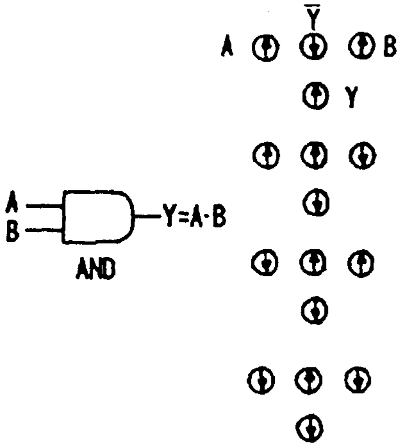


FIG. 3. The spin gate realizing the logical AND function.

$$H=\sum_{i\sigma}(\varepsilon_0 n_{i\sigma}+g\mu_B H_i \text{ sign } \sigma)+\sum_{\langle ij\rangle} t_{ij}(c^+_{i\sigma}c_{j\sigma}+\text{h.c.})+\sum_i U_i n_{i\uparrow}n_{i\downarrow}$$

$$+\sum_{\langle ij\rangle\alpha\beta} J_{ij}c^+_{i\alpha}c_{i\beta}c^+_{j\beta}c_{j\alpha}+H_z\sum_{i\sigma} g\mu_B n_{i\sigma} \text{ sign } \sigma. \tag{1}$$

The first term describes the electron energy in a single dot, H_i is the local magnetic field (along the z axis) at the ith dot, the second term describes hopping between the dots, the third term is responsible for direct Coulomb repulsion of electrons residing at the same quantum dot, the fourth term takes into account the exchange Coulomb interaction between the nearest-neighbor dots, and, finally, the last term corresponds to a uniform magnetic field which can be applied to the system. In the adopted form of the exchange interaction term, the interaction is antiferromagnetic if $J>0$, since in the subspace of states with exactly one electron at each dot it reduces to

$$\sum_{\langle ij\rangle\alpha\beta} J_{ij}c^+_{i\alpha}c_{i\beta}c^+_{j\beta}c_{j\alpha}=\sum_{\langle ij\rangle}\left(2J_{ij}\hat{S}_i\hat{S}_j+\frac{1}{4}\right).$$

For simple gates the Hamiltonian can be diagonalized numerically. Our aim is to find the range of parameters t, U, J, in which the ground state wave function (the average spin at the dots) realizes all the required states from the truth table when the local control magnetic fields are varied.

There are 6 linearly independent states for the invertor, 20 for the NAND gate, and 70 for the AND gate. The invertor Hamiltonian is a 6×6 matrix which in the basis consisting of the states

$$\left|\frac{\uparrow\uparrow}{00}\right\rangle,\ \left|\frac{\uparrow 0}{\downarrow 0}\right\rangle,\ \left|\frac{\uparrow 0}{0\downarrow}\right\rangle,\ \left|\frac{0\uparrow}{\downarrow 0}\right\rangle,\ \left|\frac{0\uparrow}{0\downarrow}\right\rangle, \text{ and } \left|\frac{00}{\downarrow\downarrow}\right\rangle$$

(in this redundant but very graphical notation the upper row corresponds to electrons with spin up, the lower to spin down, and the ith column corresponds to the ith dot) is written as

$$
\begin{array}{l|llllll|}
\left|\frac{\uparrow\uparrow}{00}\right\rangle & J+g\mu_B H_1 & 0 & 0 & 0 & 0 & 0 \\
\left|\frac{\uparrow 0}{\downarrow 0}\right\rangle & 0 & U & t & -t & 0 & 0 \\
\left|\frac{\uparrow 0}{0\downarrow}\right\rangle & 0 & t & g\mu_B H_1 & J & t & 0 \\
\left|\frac{0\uparrow}{\downarrow 0}\right\rangle & 0 & -t & J & -g\mu_B H_1 & -t & 0 \\
\left|\frac{0\uparrow}{0\downarrow}\right\rangle & 0 & 0 & t & -t & U & 0 \\
\left|\frac{00}{\downarrow\downarrow}\right\rangle & 0 & 0 & 0 & 0 & & J-g\mu_B H_1
\end{array}
$$

where we have assumed that $\varepsilon_0=0$, $t_{12}=t$, $U_1=U_2=U$, $J_{12}=J$, and H_1 is the local magnetic field at the first dot. It is useful first to consider a limiting case which allows an analytical solution and reflects the problem of state selection. Let $U=0$ and $t=0$, while $J\neq 0$ (of course, actually both $J\neq 0$ and $t\neq 0$ arise only due to the overlap of wavefunction centered at the adjacent dots). In the absence of magnetic field the wavefunction $1/\sqrt{2}(|\uparrow 0/0\downarrow\rangle - |0\uparrow/\downarrow 0\rangle)$ corresponds to the eigenstate with energy $\varepsilon=-J(J>0)$. This state has the total spin $S=0$. Apart from that, there is a triplet (total spin $S=1$) with energy $\varepsilon=J$ and wavefunctions

$$
\left|\frac{\uparrow\uparrow}{00}\right\rangle(S_z=1),\quad \left|\frac{00}{\downarrow\downarrow}\right\rangle(S_z=-1),\quad \text{and}\quad \frac{1}{\sqrt{2}}\left(\left|\frac{\uparrow 0}{0\downarrow}\right\rangle+\left|\frac{0\uparrow}{\downarrow 0}\right\rangle\right)\quad (S_z=0).
$$

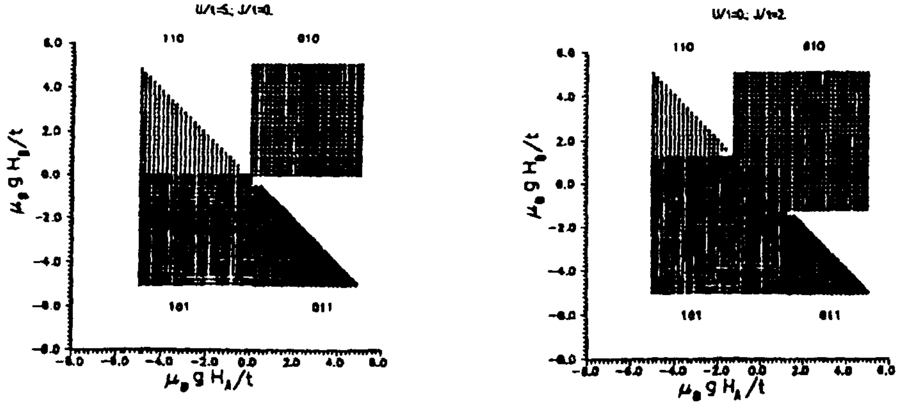
Finally, there are two more states with zero spin:

$$
\left(\left|\frac{\uparrow 0}{\downarrow 0}\right\rangle \text{ and } \left|\frac{0\uparrow}{0\downarrow}\right\rangle\right).
$$

Without the external magnetic field, the average spins on quantum dots in the ground state are zero. An external magnetic field acting on the first dot modifies the ground state energy, which becomes $\varepsilon = -\sqrt{H_1^2+J^2}$(we omit here the factor $g\mu_B$ at H_1) and induces the average spins

$$
S_1=\frac{H_1}{\sqrt{H_1^2+J^2}} \quad \text{and} \quad S_2=-\frac{H_1}{\sqrt{H_1^2+J^2}}
$$

at the input (first dot) and output (second dot), respectively. All other states have higher energies. Therefore, in the presence of the local magnetic field at the first dot the ex-



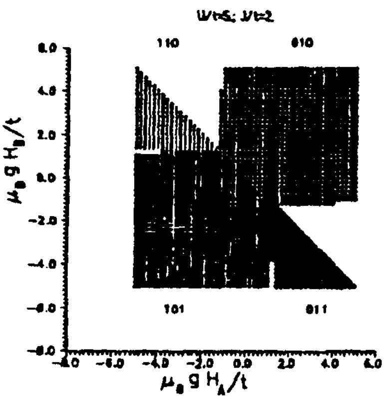


FIG. 4. Physical truth table for the spin NOT-AND gate. Cross-checked domains correspond to different lines in the truth table (the domains which can be infinitely extended to higher magnetic fields are shown only partially).

change interaction results in the appearance of average spins of equal magnitude and opposite direction on the two dots in the ground state. At arbitrary t,U,J the problem can only be solved numerically. Numerical analysis reveals no qualitative differences in the system behavior in the general case of nonzero t and U.

Consider now the less trivial example of the NAND gate, which is controlled by two input magnetic fields at dots A and B. The problem reduces to finding the domains in the plane of control magnetic fields H_A and H_B in which a particular line from the truth table is realized. The calculations were in fact performed in the following way. First the Hamiltonian spectrum and eigenvectors were found. After that the average spins S_{zi} at the dots in the ground state were calculated. To determine, for example, the range of magnetic field in which the first line in the truth table is realized, one must specify the following conditions: $S_{z1}>0$, $S_{z2}<0$, and $S_{z3}>0$. Shown in Fig. 4a is an example of the "phase diagram" for the truth table in the case $U\neq 0$, $J=0$. Different lines in the truth table of the NAND gate are realized in the corresponding magnetic field domains. An example of the "phase diagram" for $U=0$ and $J\neq 0$ is shown in Fig. 4b. For $U\neq 0$ and

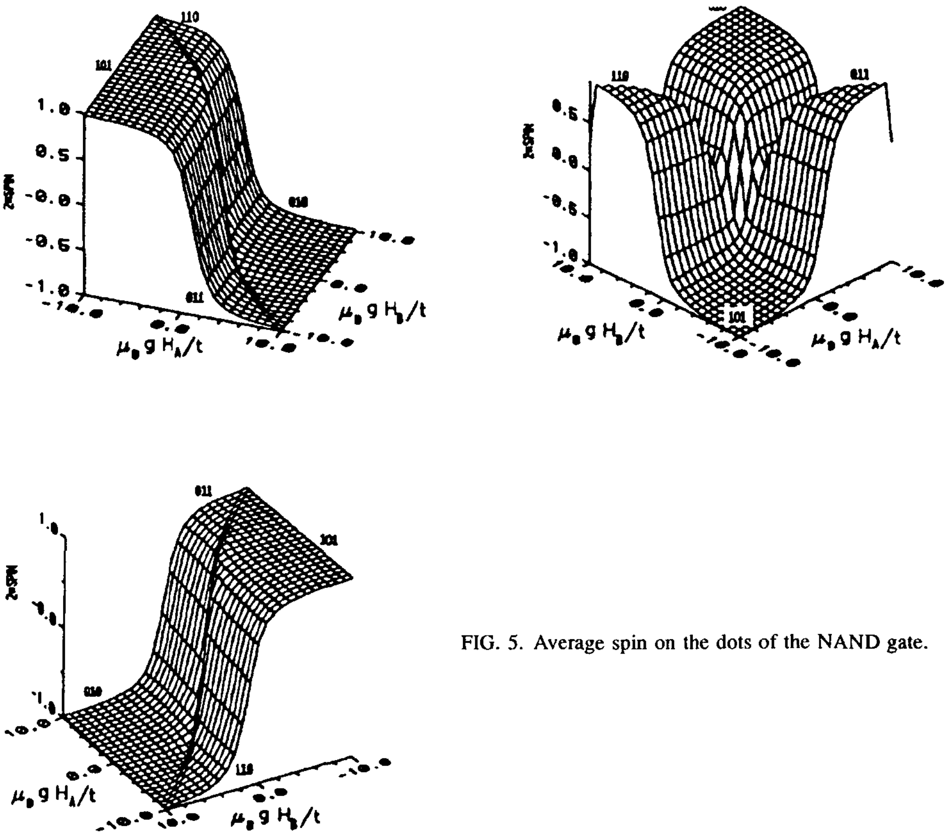


FIG. 5. Average spin on the dots of the NAND gate.

$J \neq 0$ the entire truth table can only be realized at finite control magnetic fields (Fig. 4c). In the absence of the exchange interaction all the states from the truth table can be realized at arbitrary small magnetic fields, which is more favorable from the point of view of possible experimental realization. For a finite exchange interaction the 011 and 110 states from the truth table (spin configurations $\downarrow\uparrow\uparrow$ and $\uparrow\uparrow\downarrow$, respectively) can only be realized with finite magnetic fields at the inputs. One can qualitatively understand this difference in the following way. The 101 and 010 states (spin configurations ($\uparrow\downarrow\uparrow$ and $\downarrow\uparrow\downarrow$, respectively) are energetically favorable if the exchange interaction is antiferromagnetic, tending to align adjacent spins antiparallel, so that an arbitrarily small magnetic field lifting the degeneracy between these states is sufficient to select one of these configurations. In that sense both $\downarrow\uparrow\uparrow$ and $\uparrow\uparrow\downarrow$ configurations are unfavorable since the spins at the adjacent dots are parallel rather than antiparallel, increasing the exchange interaction contribution to the system energy. Therefore, a finite magnetic field is needed in order to realize these states. If only the intradot Coulomb repulsion is included in the Hamiltonian, there is no such threshold in the magnetic field (although the Coulomb repulsion is known to result in antiferromagnetic correlations of the spins at adjacent sites, the system turns out to be "softer" in this case).

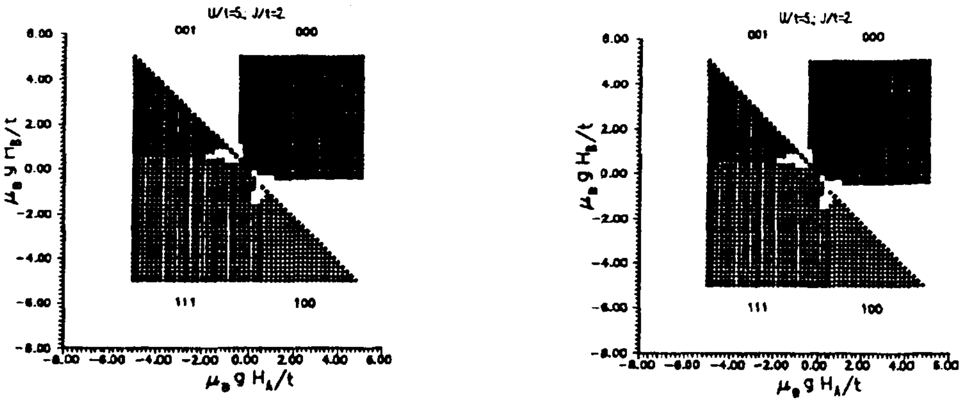


FIG. 6. Physical truth table for the spin AND gate.

We have also analyzed systems with a ferromagnetic exchange interaction and nonzero intradot Coulomb repulsion. The truth table was also found to be realizable in that case, although at finite magnetic fields only. The threshold in magnetic field in the case of nonzero exchange interaction is not eliminated by a uniform magnetic field either.

It is also interesting to trace the spin values at different magnetic fields. The average spin polarizations at the dots of the NAND gate $[S_{zi}(H_A, H_B)]$ are shown in Fig. 5 for $U/t=5$, $J/t=2$ as functions of the local control magnetic fields. It is seen that for favorable configurations of adjacent spins their values saturate [approaching $S_z=1/2$)] at low magnetic fields. At the same time, in the domains where the adjacent spins are parallel, the limiting values at high magnetic fields do not reach $S_z=1/2$.

Calculations performed for the AND gate, too, reveal that the entire truth table can also be realized at appropriate system parameters. As in the preceding case, all the states from the truth table can be realized at arbitrarily small magnetic fields only in the presence of a strong enough intradot Coulomb repulsion (Figs. 6a,b).

A crucial point for the physical realization of complex gates is the length at which the electron–electron interaction can maintain the required spin configuration. If the output is far enough from the inputs (is separated from them by a large number of quantum dots) and the input spins are close to 1/2, one cannot be sure that the spin amplitude will not decay far from the outputs. In the general case the answer is not known. However, in the case of the AND gate it is clearly seen from Fig. 7 that the interaction induces a spin of the same magnitude (but antiparallel) at the direct output as at the inverted one. Therefore, one can hope that the interaction will be able to maintain the spin amplitude at larger distances from the inputs as well. However, Fig. 7 reveals that for energetically unfavorable configurations the average spin is rather small, which may be a serious obstacle to experimental realization of the gates. In addition, since all the structures are one- or at best two-dimensional, one can expect the magnetic ordering induced by the input control magnetic field to vanish for sufficiently large sizes of the gates. Unfortunately, we are currently unable to calculate the critical system size.

To summarize, by analyzing the simplest logical gates we have established that:

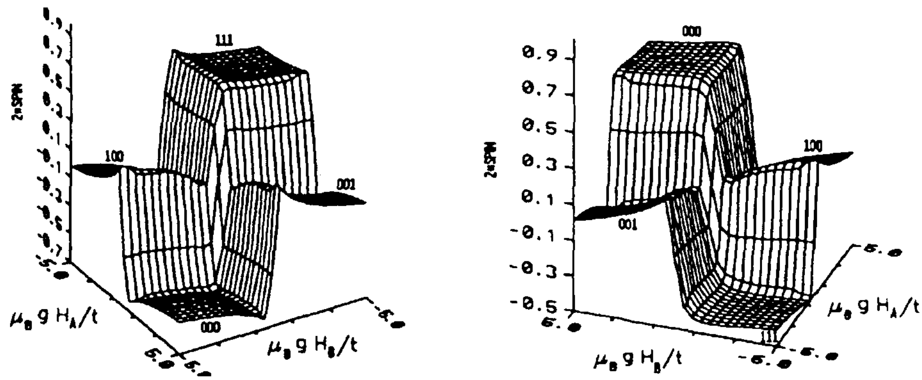


FIG. 7. Average spin at the direct and inverse outputs of the spin AND gate.

1) in the presence of only intradot Coulomb repulsion the entire truth table can be realized at arbitrarily small magnetic fields at the input dots;

2) in the presence of an exchange interaction the truth table can only be realized at finite input magnetic fields (a typical threshold field here corresponds to the exchange interaction energy);

3) at least for small gates, the electron–electron interaction can maintain the required spin configuration through the intermediate quantum dots.

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