

# Switching in a reversible spin logic gate

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Theoretical results for the adiabatic switching of a reversible quantum inverter—realized with two antiferromagnetically coupled single electrons in adjacent quantum dots—are presented. It is found that a large exchange interaction between the electrons favors faster switching but also makes the timing of the read cycle more critical. Additionally, there exists an optimal input signal energy to achieve complete switching. Only for this optimal signal energy does the inverter yield an unambiguous, logically definite state. An experimental strategy for realizing circuits based on such gates in self-assembled arrays of quantum dots is briefly discussed.

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#### 1. Introduction

Research in nanoelectronic classical Boolean logic circuits derived from single electron interactions in quantum dots has been a busy field for the last few years [1–9]. A number of ideas have appeared in the literature [1–9] that visualize building dissipative (non-reversible) logic circuits based on Coulomb or exchange interaction between single electrons in arrays of quantum dots. Some of these schemes (e.g. [2]), however, are not only flawed, but they also violate the basic tenets of circuit theory. The individual logic devices have no isolation between input and output so that the input bit cannot even uniquely determine the output bit! (for a discussion of this issue see [3–6, 10]).

In this paper, we explore a different type of gate. It is a quantum mechanical gate that is reversible and non-dissipative. It should be contrasted with 'parametron-type' constructs that dissipate less than  $kT \ln 2$  energy per bit operation [11], but are otherwise not entirely non-dissipative. While the bits in a parametron are c-numbers, the bits in the quantum gate to be described are true qubits and the time evolution of the system is unitary. For the sake of simplicity, we consider the smallest quantum gate possible, namely an inverter. It is fashioned from two antiferromagnetically coupled single electrons in two closely spaced quantum dots as envisioned in [3–5]. The equilibrium steady-state behavior of such a system has been investigated by Molotkov and Nazin [7, 8]. Here, we will explore the dynamic behavior and the unitary time evolution of this system in a non-dissipative and globally phase-coherent environment.

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**Fig. 1.** Two adjacent quantum dots hosting single electrons. In the ground state, the spins of the two electrons are antiparallel. If spin polarization is used to encode binary bits, the logic state of one dot is always the inverse of the other. This realizes an inverter in which one dot acts as the input terminal and the other as the output.

## 2. Theory

Consider two single electrons housed within two closely-spaced quantum dots as shown in Fig. 1. It was shown in [3] that the preferred ordering of this system is antiferromagnetic, i.e. the two electrons have opposite spins. If the spin polarization in one dot is considered to be the input 'qubit' and that in the other the output 'qubit', then this system acts as an inverter since the spin-polarizations are antiparallel (logic complement) [3, 8]. Note that an inverter is always logically reversible since one can invariably predict the input bit from a knowledge of the output bit (in practice, the input bit is recovered by merely passing the output through another inverter). However, such a gate is not a universal quantum gate unlike the Toffoli gate [12]. Various schemes for realizing non-dissipative and reversible quantum logic gates have recently appeared in the literature [13–18]. Experimental demonstrations of quantum logic gates have also been reported [19, 20]. Almost all of these schemes encode the qubit in a photon (rather than an electron) state thereby requiring optical components that are incompatible with ultra-large-scale integration. In contrast, the spin gate based on single electrons in quantum dots is very appealing from the perspective of high-density circuits.

To analyse the system in Fig. 1 quantum-mechanically, we will assume that there is only one size-quantized level in each quantum dot. Then, the Hubbard Hamiltonian for this system in the presence of a globally applied magnetic field can be written following Molotkov and Nazin [7] as

$$\mathcal{H} = \sum_{i\sigma} (\epsilon_0 n_{i\sigma} + g \mu_{\rm B} H_i \operatorname{sign}(\sigma)) + \sum_{\langle ij \rangle} t_{ij} (c_{i\sigma}^+ c_{j\sigma} + h.c.) + \sum_i U_i n_{i\uparrow} n_{i\downarrow}$$

$$+ \sum_{\langle ij \rangle \alpha\beta} J_{ij} c_{i\alpha}^+ c_{i\beta} c_{j\beta}^+ c_{j\alpha} + H_z \sum_{i\sigma} g \mu_{\rm B} n_{i\sigma} \operatorname{sign}(\sigma)$$

$$(1)$$

where the first term denotes the electron energy in the ith dot ( $H_i$  is a z-directed local magnetic field selectively applied at the ith dot), the second term denotes the hopping between dots, the third term is the Coulomb repulsion within the ith quantum dot, the fourth term is the exchange interaction between nearest-neighbour dots and the last term is the Zeeman splitting energy corresponding to the globally applied magnetic field oriented along the z-direction.

We can simplify the Hamiltonian in Eqn (1) to the Heisenberg model following Molotkov and Nazin [8] to yield

$$\mathcal{H} = J \sum_{\langle ij \rangle} \sigma_{zi} \sigma_{zj} + J \sum_{\langle ij \rangle} (\sigma_{xi} \sigma_{xj} + \sigma_{yi} \sigma_{yj}) + \sum_{\text{input dots}} \sigma_{zi} h_{zi}^{\text{input}} \qquad (J > 0)$$
 (2)

where we have neglected the global magnetic field. The quantity  $h_{zi}^{\text{input}}$  is the Zeeman energy caused by a local magnetic field applied to the *i*th dot in the *z*-direction which will orient the spin in the *i*th dot along that field. Such a local field can be applied via a spin-polarized scanning tunneling microscope (SPSTM) tip as visualized in [3] and serves to provide an input signal to the gate.

**Table 1:** Eigenenergies and eigenstates of the Hamiltonian for an inverter.

Eigenenergies	Eigenstates
$h_A + J$	$ \downarrow\downarrow angle$
$-J + \sqrt{h_A^2 + 4J^2}$	$\sqrt{\frac{1}{2}\left(1+\frac{h_A}{\sqrt{h_A^2+4J^2}}\right)} \uparrow\downarrow\rangle+\sqrt{\frac{1}{2}\left(1-\frac{h_A}{\sqrt{h_A^2+4J^2}}\right)} \downarrow\uparrow\rangle$
$-J - \sqrt{h_A^2 + 4J^2}$	$\sqrt{\frac{1}{2}\left(1 - \frac{h_A}{\sqrt{h_A^2 + 4J^2}}\right)} \uparrow\downarrow\rangle - \sqrt{\frac{1}{2}\left(1 + \frac{h_A}{\sqrt{h_A^2 + 4J^2}}\right)} \downarrow\rightarrow\rangle$
$-h_A+J$	$ \uparrow\uparrow\rangle$

In the basis of states  $|\sigma_A \sigma_B\rangle$  (A and B are the two electrons), the Hamiltonian in Eqn (2) can be written as

$$\begin{pmatrix} h_A + J & 0 & 0 & 0 \\ 0 & h_A - J & 2J & 0 \\ 0 & 2J & -h_A - J & 0 \\ 0 & 0 & 0 & -h_A + J \end{pmatrix}$$
 (3)

where  $h_A$  is the interaction with the input magnetic field selectively applied to quantum dot A. The twoelectron basis states can be denoted as  $|\downarrow\downarrow\rangle$ ,  $|\uparrow\downarrow\rangle$ ,  $|\downarrow\uparrow\rangle$  and  $|\uparrow\uparrow\rangle$ ; they form a complete orthonormal set. The 'upspin' polarization is oriented along the direction of the locally applied external magnetic field in this representation.

The eigenenergies and corresponding eigenvectors of the above Hamiltonian are given in Table 1.

It is obvious that the third row in Table 1 corresponds to the ground state. In the absence of any external magnetic field  $(h_A = 0)$ , the ground-state energy is -3J and the ground-state wavefunction is  $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)$ . note that the ground state in the absence of any external magnetic field is an entangled state in which neither the quantum dot A nor the quantum dot B has a definite spin polarization.

## 3. Adiabatic switching

We now wish to study the following switching problem. Assuming that the inverter is in its ground state without any applied magnetic field, we will calculate how long it takes after a magnetic field is applied to quantum dot A for the spin in A to orient along the field and the spin in B to orient in the opposite direction (as required by the inversion operation).

After the external field is applied at time t=0, the inverter evolves in time according to the unitary operation

$$[c(t)] = \exp[-i\mathcal{H}t/\hbar][c(\mathbf{0})] \tag{4}$$

where  $\mathcal{H}$  is given by Eqn (3) and [c] is a four-element unit vector  $[c_1, c_2, c_3, c_4]$  that describes the wavefunction  $\psi(t)$  according to

$$\psi(t) = c_1(t)|\downarrow\downarrow\rangle + c_2(t)|\uparrow\downarrow\rangle + c_3(t)|\downarrow\uparrow\rangle + c_4(t)|\uparrow\uparrow\rangle. \tag{5}$$

The initial conditions are described by

$$\begin{bmatrix} c_1(0) \\ c_2(0) \\ c_3(0) \\ c_4(0) \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}.$$
 (6)

The solution of Eqn (4) subject to the initial condition given by Eqn (6) is

$$c_{1}(t) = c_{4}(t) = 0$$

$$c_{2}(t) = \frac{e^{iJt/\hbar}}{\sqrt{2}} \left[ \cos(\omega t) - i \left( \frac{h_{A}}{\hbar \omega} + \sqrt{1 - \frac{h_{A}^{2}}{\hbar^{2} \omega^{2}}} \right) \sin(\omega t) \right]$$

$$c_{3}(t) = -\frac{e^{iJt/\hbar}}{\sqrt{2}} \left[ \cos(\omega t) - i \left( \frac{h_{A}}{\hbar \omega} - \sqrt{1 - \frac{h_{A}^{2}}{\hbar^{2} \omega^{2}}} \right) \sin(\omega t) \right]$$
(7)

where  $\omega = \sqrt{h_A^2 + 4J^2}/\hbar$ .

Therefore, the wavefunction at an arbitrary time t is given by

$$c_2(t)|\uparrow\downarrow\rangle + c_3(t)|\downarrow\uparrow\rangle \tag{8}$$

with  $c_2$  and  $c_3$  given by Eqn (7).

After the switching is complete, the system should be in the state  $|\uparrow\downarrow\rangle$ . Therefore, the switching delay  $t_{\rm d}$  can be defined as the time taken for  $|c_2(t)|$  to reach its maximum value and, correspondingly, for  $|c_3(t)|$  to reach its minimum value.

This yields

$$t_{\rm d} = \frac{h}{4\sqrt{h_A^2 + 4J^2}}. (9)$$

It should be understood that the system *does not* reach a steady state at time  $t = t_d$ , but instead continues to evolve in accordance with Eqn (4). The computation (inversion) can be halted by reading the spin-polarization (logic bit) in the output dot (dot B) with a SPSTM tip at time  $t = t_d$  since the reading operation is dissipative and collapses the wavefunction. Note that the higher the frequency  $\omega$ , the more critical is the timing for the read cycle that halts the quantum computation. Since  $\omega$  increases with the exchange energy J, a larger J will mandate a greater accuracy in the read cycle.

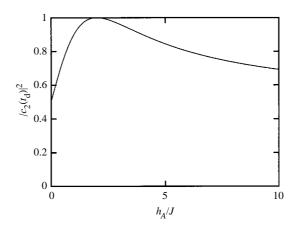
To achieve complete switching, the magnitude  $|c_2(t_d)|$  should be unity and  $|c_3(t_d)|$  should vanish. From Eqns (7) and (9), we obtain

$$|c_2(t_d)| = \frac{h_A + 2J}{\sqrt{2h_A^2 + 8J^2}}. (10)$$

The magnitude  $|c_2(t_d)|^2$  as a function of the normalized input signal energy  $h_A/J$  is shown in Fig. 2. It reaches a maximum value of unity (corresponding to complete switching) when  $h_A = 2J$ . Therefore, there exists an optimal value of the input signal energy  $h_A$  for which complete switching can be obtained.

It should be noted from Eqn (9) that the switching delay decreases with increasing exchange energy J. For the optimal case  $(h_A=2J)$ , the switching delay is  $h/(8\sqrt{2}J)$ . We can estimate the order of magnitude for  $t_{\rm d}$ . Presumably, the maximum value of local magnetic field that can be applied to a dot with a SPSTM tip is about 1 T. Since  $h_A\approx g\mu_{\rm B}B$  ( $\mu_{\rm B}$  is the Bohr magnetron), this means that the maximum value of  $h_A$  that we can hope to obtain is about 0.1 meV if we assume the Landé g-factor to be 2. Consequently,  $J_{\rm optimal}=0.05$  meV. This gives a value of  $t_{\rm d}\approx 7$  ps. Therefore, these inverters are capable of quite fast switching.

We can also estimate the temperature of operation for such inverters. Since the exchange energy should exceed the thermal energy kT for stable operation, the ambient temperature should be restricted to below T=J/k=570 mK. Because the operation of the inverter requires global phase coherence (i.e. the phase breaking time should be significantly longer than  $t_{\rm d}$ ), a low temperature is also otherwise required. To increase the temperature to a more practical value of 4.2 K,  $J_{\rm optimal}$  should be 0.364 meV and therefore  $h_A$  should be as large as 0.728 meV. This requires the ability to generate a local magnetic flux density in excess of 7 T with an SPSTM tip as an input to cell A. This is not possible with present state of SPSTM technology, but could become feasible in the future.



**Fig. 2.** The magnitude of  $|c_2(t_d)|^2$  as a function of the normalized unput signal energy  $h_A/J$ .

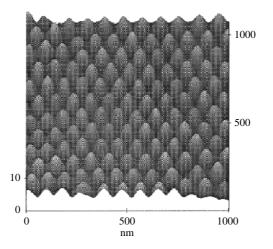


Fig. 3. Atomic force micrograph of a self-assembled mask to create a periodic array of quantum dots. Details can be found in [4,6].

We conclude this paper with a brief discussion of experimental strategies undertaken by us in our efforts to fabricate such gates. We believe that the optimal technique is 'gentle' self-assembly of quantum dots rather than nanolithography which causes processing damage and has a slow throughput. We fabricate a regular array of the dots using a self-assembled mask for mesa-etching. The self-assembled mask is created by evaporating aluminum on the chosen semiconductor structure and then electropolishing it in a solution of perchloric acid, butyl cellusolve and ethanol at 60 V for 30 s at room temperature. Figure 3 shows the raw atomic force micrograph of a self-assembled mask of aluminum with a dimpled surface that consists of a periodic array of crests and troughs with hexagonal packing. The troughs are etched away by an appropriate etchant leaving a regular pattern of isolated crests on the surface of the semiconductor structure that serve as a mask through which mesas are etched. Owing to space limitations, we will omit details of the fabrication process, but instead refer the reader to [4, 6].

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