A BISTABLE QUANTUM CELL FOR CELLULAR AUTOMATA

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Abstract

We investigate the behavior of few-electron systems consisting of tightly-coupled quantum dots. Specifically, we concentrate on a model cell which consists of five quantum dots occupied by two electrons. The mutual Coulombic repulsion, quantum confinement, and discrete nature of the electronic charge, lead to cell states which exhibit distinct charge alignments. Electrostatic coupling between neighboring cells is shown to result in bistable saturation of the cell polarization. Implications of this bistability for quantum cellular automata are discussed.

INTRODUCTION

Various investigators have pointed out the natural link between mesoscopic quantum systems and cellular automata (CA) architectures [1]. Because quantum structures are necessarily so small it is difficult to conceive of a regime in which a single quantum device could drive many other devices in subsequent stages [2]. Furthermore, the connections between devices would tend to dominate the behavior of the assembly of devices. For these reasons locally interconnected structures such as cellular neural networks and cellular automata may provide the natural architecture for quantum devices.

A quantum cellular automaton would consist of an array of cells, each of which is some sort of quantum nanostructure. For a two-state CA, each cell should have two stable quantum states. The state of a given cell should influence the state of the neighboring cells. Two ingredients are essential then: 1) the bistability of the cell, and 2) coupling to neighboring cells.

We examine a paradigm in which the cell itself is composed of coupled quantum dots [3] occupied by two electrons. The bistability is accomplished through the interaction of 1) quantum confinement effects, 2) the Coulomb interaction between the two electrons, and 3) the quantization of charge (as in the Coulomb blockade). The intercellular interaction is provided by the Coulomb repulsion between electrons in different cells.

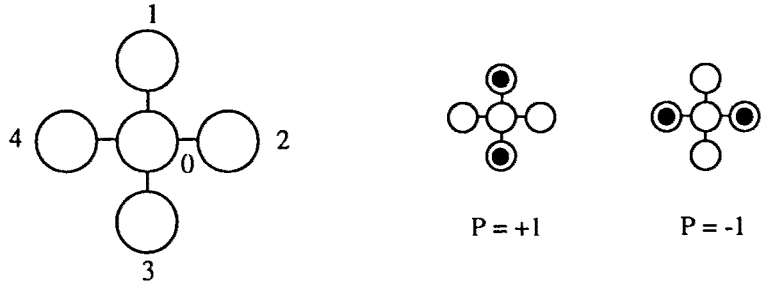

FIGURE 1. A quantum cell with 2 electrons.

The specific cell we consider here is shown in Figure 1. Four quantum dots are coupled to a central dot by tunnel barriers. The two electrons tend to occupy antipodal sites in one of two configurations, shown in the figure as the P=+1 and P=-1 configurations. Our analysis below will show that the cell is indeed in one of these two stable states, and that an electrostatic perturbation, perhaps caused by neighboring cells, switches the cell between these two states in a very abrupt and nonlinear way.

MODEL

We have calculated the response of the cell to perturbations in the electrostatic potential at the sites using a Hubbard-type Hamiltonian. For the isolated cell, the Hamiltonian can be written,

$$H_0^{cell} = \sum_{i,\sigma} E_0 n_{i,\sigma} + \sum_{i,\sigma} t\,(a_{i,\sigma}^{\dagger} a_{0,\sigma} + a_{0,\sigma}^{\dagger} a_{i,\sigma}) + \sum_{i} E_Q n_{i,1} n_{i,2} + \sum_{i>j,\sigma,\sigma'} V_Q(i,j)\, n_{i,\sigma} n_{i,\sigma'}$$

Here $a_{i,\sigma}$ is the annihilation operator which destroys a particle at site i with spin σ (σ= *1* or *2* indicates spin up or down). The number operator for site i and spin σ is represented by $n_{i,\sigma}$. The on-site energy for each dot is E_0; the tunneling amplitude to the central dot is t; the charging energy for a single dot is E_Q, and the Coulombic potential energy for electrons at sites i and j is $V_Q(i,j)$.

The effect of neighboring cells is modeled very simply by a change in the on-site potential for one dot only - the dot labeled 2 in Figure 1. Thus if

$$V = \sum_{\sigma} E_0 n_{2,\sigma}$$

then the total Hamiltonian is

$$H^{cell} = H_0^{cell} + \alpha V$$

where α is a parameter which determines the strength of the perturbation. The cell Hamiltonian is diagonalized directly in the basis of two-electron states [4]. We can thereby calculate directly the ground-state two-electron wavefunction.

It is useful to define a quantity which represent the degree to which a given eigenstate of the system consists of electrons aligned vertically or horizontally. For each site, we calculate the single particle density ρ_i, which is simply the expectation value the total number operator for the two-electron eigenstate. The polarization, P, is defined as

$$P = \frac{(\rho_1 + \rho_3) - (\rho_2 + \rho_4)}{\rho_0 + \rho_1 + \rho_2 + \rho_3 + \rho_4}$$

The polarization thus defined is not to be confused with the usual dipole polarization of a continuous medium. It simply represents the degree to which the electrons in the cell are aligned and in which of the two possible directions the alignment occurs. For the states of interest here, the cell is an electrostatic quadrupole with no dipole moment

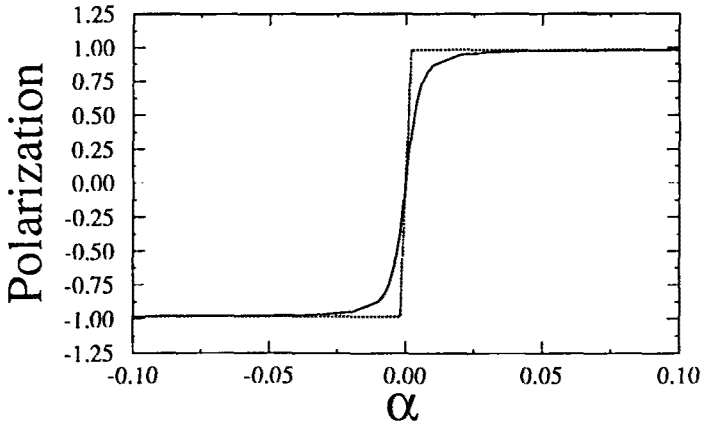

FIGURE 2. Polarization of the lowest-energy cell eigenstate. The solid curve is for the singlet spin state and the dashed curve is for the triplet spin state.

RESULTS

We solve the time independent Schrödinger equation using H^{cell} above for various values of the perturbation parameter α. For each value of α, we calculate ground-state single particle densities, ρ_i, and the resultant polarization *P*. For $\alpha=0$, the isolated cell, the ground-state is a degenerate combination of both polarization, $P=+1$ and $P=-1$, with no polarization preferred.

The ground-state polarization is shown in Figure 2 as a function of α. The solid line is for the spin-singlet, spatially symmetric state and the dashed line is for the spin-triplet, spatially antisymmetric state. Both show the strong abrupt bistability of the polarization. Even a very small asymmetry in the potential induces a strongly saturated polarization. For the spin-triplet case, the response is indistinguishable from a step-function.

The eigen-energies for the lowest two eigenstates is shown in Figure 3. Energies for both the singlet and triplet spin states are shown. To be of use in a CA-type design, the energy splitting between the ground-state and the first excited state (which have opposite polarizations) must be larger than the thermal energy k_BT.

The nonlinear bistable saturation [5] evident from this calculation makes it clear that this type of cell is a good candidate for CA architectures. We have begun modeling arrays and systems of such cells. The CA rules for a regular array can be generated from the cell Hamiltonian as follows. For each combination of near-neighbor polarizations, find the potential on each site of the central cell. Solve the two-electron Schrödinger equation with that potential and calculate the polarization of the ground state. This process produces a table of CA rules sufficient to completely determine CA behavior. Note that because the ground-state properties are always employed, dissipation is assumed in the model [6].

In conclusion, we have identified a model nanostructure which we believe is an excellent candidate for forming the basis of quantum cellular-automata (CA) arrays. It consists of a central quantum dot and four neighboring dots occupied by two electrons [7]. The Coulomb repulsion between the two electrons, quantum confinement effects, and the discreteness of the electronic charge, combine to produce strongly polarized (in the sense defined above) ground states. The response of this polarization to the electrostatic environment is highly nonlinear and exhibits the bistable saturation necessary for a two-state CA.

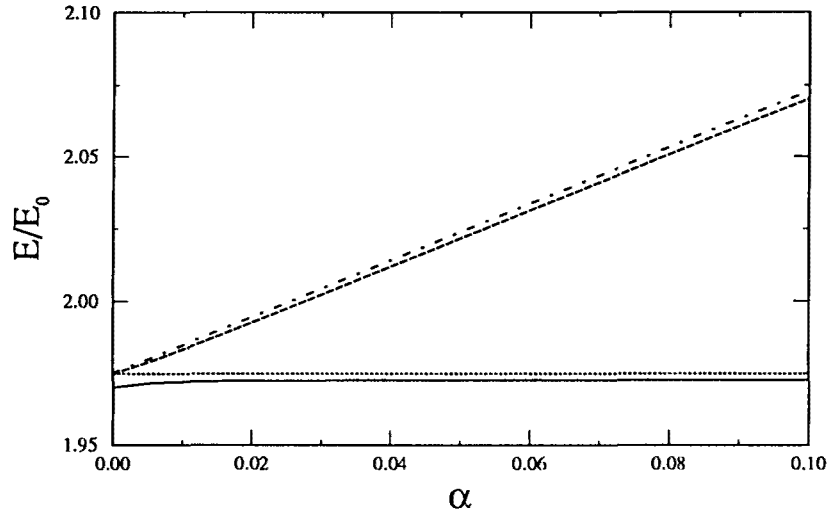

FIGURE 3. Energies of the two lowest-energy cell eigenstates. The solid and dot-dashed curves are for the singlet spin state. The dashed and dotted curves are for the triplet spin state.

ACKNOWLEDGEMENTS

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REFERENCES

1. R. T. Bate, *Bull. Am. Phys. Soc.* **22**, 407 (1977); and D. K. Ferry, L. A. Akers, and E. W. Greeneich, *Ultra Large Scale Interconnected Microelectronics* (Prentice Hall, Englewood Cliffs N.J., 1988); J.N. Randall, M.A. Reed, and G.A. Frazier, *J. Vac. Sci. Technol.* **B7**, 1398, (1989).

2. R. Landauer, *Phys. Today* **42**, 119 (1989).

3. B. Meurer, D. Heitmann, and K. Ploog, *Phys. Rev. Lett.* **68**, 1371 (1992).

4. Craig S. Lent, *Nanostructures and Mesoscopic Systems*, Wiley P. Kirk and Mark A. Reed (eds.), 183 (Academic Press, Boston, 1992).

5. K. Obermayer, G. Mahler, and H. Haken, *Phys. Rev. Lett.* **58**, 1792 (1987).

6. Craig S. Lent, P. Douglas Tougaw, and Wolfgang Porod, unpublished.

7. Cells with single electron occupancy are discussed by P. Bakshi, D.A. Broido, and K. Kempa, *J. Appl. Phys.* **70**, 5150 (1991).