Bistable saturation in coupled quantum dots for quantum cellular automata

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A simple model quantum dot cell containing two electrons is analyzed as a candidate for quantum cellular automata implementations. The cell has eigenstates whose charge density is strongly aligned along one of two directions. In the presence of the electrostatic perturbation due to a neighboring cell, the ground state is nearly completely aligned (polarized) in one direction only. The polarization is a highly nonlinear function of the perturbing electrostatic fields and shows the strong bistable saturation important for cellular automation function.

Nanoscale quantum structures with potential device applications have been an active area of exploration for several years. A frequent criticism[1] of many of these structures is the absence of the saturating behavior which forces conventional transistor elements into one of two stable states, "on" or "off." Such bistable saturation is important to keep device performance robust in the presence of physical inhomogeneities and noise.[2]

The possibility of realizing cellular automata (CA) with regular arrays of quantum dots has been suggested by Bate and others.[3] In one example, the necessary nonlinear response of each dot is the result of resonant tunneling through the dot.[4] We focus on a different paradigm in which each cell of the CA is composed of groups of coupled quantum dots. The confining potentials are such that electrons can tunnel between dots in the same cell but not between different cells. Quantum mechanics and the Coulomb interaction in each cell determine the possible cell states. The Coulomb interaction between electrons in different cells provides a local intercellular coupling mechanism. The nonlinear response of the cell to its electrostatic environment must be a feature of the internal cell dynamics. Recent success in fabricating arrays of very small quantum dots with one or two electrons per dot[5] prompts us to investigate possible few-electron coupled-dot cell geometries which provides the sort of bistable saturation so desirable. In this letter, we analyze a possible cell geometry with two electrons in the cell. We show that quantum confinement and the intracellular Coulomb interaction together yield the nonlinear saturation behavior which is essential.

We examine a simple nanostructure model cell containing five coupled quantum dots. The model cell is shown schematically in Fig. 1. It consists of a central site and four neighboring sites. Tunneling is possible both between the outer sites and the central site, and between adjacent outer sites. We first consider such a cell holding two electrons (the contrasting case of single and triple cell occupancy is discussed below). We show below that the Coulomb repulsion between the two electrons causes the ground state of the system to be one in which the electrons occupy antipodal sites.

We model the cell using a Hubbard-type Hamiltonian with Coulomb repulsion. The Hamiltonian for a single isolated cell can be written,

$$H_0^{\text{cell}} = \sum_{i,\sigma} E_0 n_{i,\sigma} + \sum_{i,j,\sigma} t_{i,j}(a_{i,\sigma}^{\dagger} a_{j,\sigma} + a_{j,\sigma}^{\dagger} a_{i,\sigma}) + \sum_{i} E_Q n_{i,\uparrow} n_{i,\downarrow} + \sum_{i>j,\sigma,\sigma'} V_Q \frac{n_{i,\sigma} n_{j,\sigma'}}{|r_i - r_j|}, \quad (1)$$

where the number operator $n_{i,\sigma} = a_{i,\sigma}^{\dagger} a_{i,\sigma}$ and the operator $a_{i,\sigma}^{\dagger}$ creates an electron at site i with spin σ. The cell parameters which define the Hamiltonian are then the on-site energy, E_0, the tunneling energies, $t_{i,j}$, and the on-site Coulomb charging energy, E_Q. The parameter V_Q is determined by fundamental constants and the dielectric constant of the material in which the dots are formed. A fixed positive charge $\tilde{\rho}$ is assumed at each site sufficient to maintain overall cell charge neutrality. For an isolated cell, this only renormalizes E_0, but it is important in calculating the interaction between cells as is done below.

For the numerical results we discuss here we choose parameters based on a simple, experimentally accessible model. We consider a cell in a semiconductor with $m^* = 0.067 m_0$, which is composed of circular quantum dots of diameter $D = 10$ nm. The near-neighbor distance between the cells is 20 nm. The dielectric constant for the semiconductor is 10. We take $t = 0.3$ meV for coupling to the center site and $t = 0.03$ meV for coupling between outer dots. These tunneling energies can be varied greatly by adjusting the potential barriers between dots. We take $E_Q = V_Q/(D/3)$. We will assume here that the two electrons in the cell have antiparallel spins. The parallel spin case yields results which are qualitatively very similar.

The eigenstates of the Hamiltonian [Eq. (1)] can now be calculated for this specific choice of cell parameters. The Hamiltonian is diagonalized directly in the basis of few-electron states. From the two-electron wave function we calculate the single particle density at each site, ρ_i by find-

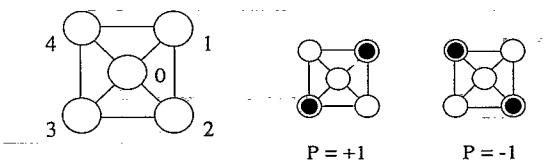

FIG. 1. The quantum cell consisting of five quantum dots which are occupied by two electrons. The mutual Coulomb repulsion between the electrons results in bistability between the $P = +1$ and $P = -1$ states.

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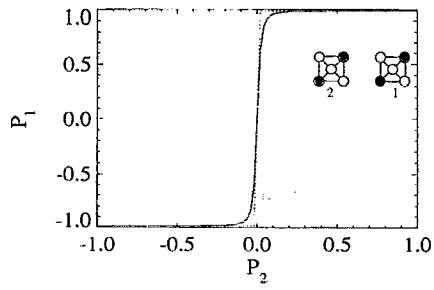

FIG. 2. The cell-cell response function. The induced polarization of cell 1 is shown as a function of the polarization in a neighboring cell 2 (inset). The solid line represents the polarization of the ground state and the dashed line represents the polarization of the first excited state.

ing the expectation value of the total number operator, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, at each site.

It is helpful to define a scalar quantity which represents the degree to which the electron density is aligned either along the line through sites 1 and 3, or along the line through sites 2 and 4. To this end we define the polarization of the cell as

$$P = \frac{(\rho_1 + \rho_3) - (\rho_2 + \rho_4)}{\rho_0 + \rho_1 + \rho_2 + \rho_3 + \rho_4}. \tag{2}$$

If sites 2 and 4 are vacant, the cell is completely in the $P = +1$ polarized state as shown in Fig. 1. If sites 1 and 3 are vacant, the cell is completely in the $P = -1$ polarized state. Clearly if the on-site energies are the same for all sites, the ground state is degenerate, comprising a combination of both polarizations, with no polarization preferred.

We examine the polarization of the low-lying eigenstates of the cell when perturbed by the presence of a nearby cell. We denote the target cell as cell 1 and the perturbing cell as cell 2. The potential at each site i of cell 1 is altered by the Coulomb interaction with the charge $\rho_{2,j}$ at site j of cell 2. The Hamiltonian for cell 1 can be written as the sum of the isolated cell Hamiltonian and a perturbation due to cell 2.

$$H^{\text{cell}} = H_0^{\text{cell}} + H_{12}^{\text{cell}}, \tag{3}$$

where

$$H_{12}^{\text{cell}} = \sum_{i,j,\sigma} V_Q \frac{\rho_{2,j} - \tilde{\rho}}{|\mathbf{R}_{2,j} - \mathbf{R}_{1,i}|} n_{i,\sigma}. \tag{4}$$

Here $R_{m,i}$ denotes the position of site i in cell m. We solve for the eigenstates of the Hamiltonian [Eq. (3)] as the polarization of cell 2 is varied in the range $P_2 = [-1, 1]$. The occupancy of the central site in cell 2 is assumed to be zero[6] so that the charge densities, $\rho_{2,j}$, are simple functions of the polarization P_2. The distance between cell centers is three times the near-neighbor distance in a cell. For each value of P_2, we find the eigenstates and the associated charge densities and polarizations (Eq. 2). The result is the cell-cell response function—the polarization of cell 1 induced by a polarization of cell 2.

Figure 2 shows the polarization P_1 of the lowest two cell eigenstates as a function of the perturbing cell polarization P_2. This figure displays the central result of this letter—that the cell-cell response function is highly nonlinear and bistable. Even a very slight polarization of a cell induces nearly complete polarization of a neighbor.

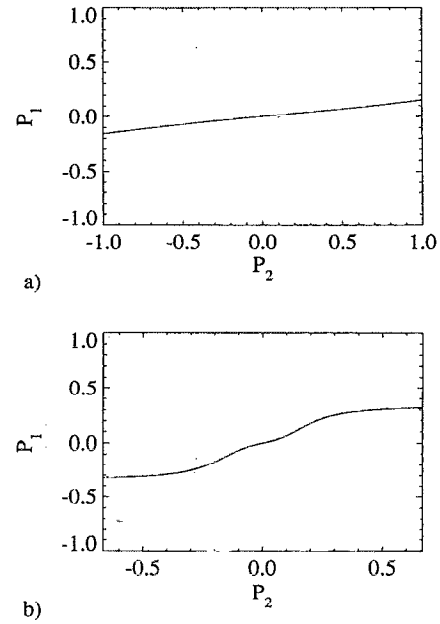

FIG. 3. The cell-cell response function for other cell occupancies. (a) A single electron in the cell. (b) Three electrons (two spin up and one spin down) in the cell.

The strongly nonlinear saturation of the polarization does not occur if only a single electron is in the cell.[7] Figure 3(a) shows the cell-cell response function for the ground state of a cell occupied by a single electron. The polarization is a very weak and nearly linear function of the perturbation.[8] The response function for a triply occupied cells (two spin up, one spin down) is shown in Fig. 3(b). Although the response is clearly not linear, it is not nearly as strong as the two-electron case. The bistable saturation present in the doubly occupied cells is a result of the distinct splitting of the degenerate ground state by the perturbation of a neighboring cell.

The rapid saturation of the polarization is the essential nonlinear effect which suggests this type of cell could provide the basis for a CA-type array. In such an array of cells, the differing polarizations of neighboring cells would provide the electrostatic perturbation which leads to a definite polarization of the ground state of the cell. It is possible to extract a CA rule set by finding the cell polarization induced from the various combinations of neighboring polarizations. This process, and the behavior of arrays of quantum cells will be discussed at greater length elsewhere.[9]

It must be noted that to date, quantum dot fabrication techniques have produced dots which tend to be rather far apart, thus only rather weak Coulombic coupling exists.[4] Our analysis presumes that fabrication techniques will shortly overcome these difficulties, possibly through macromolecular rather than semiconductor implementations.[10]

In conclusion, we have shown that strongly nonlinear saturation effects occur in a model two-electron nanoscale system. The charge density "snaps" into one of two positions, depending sensitively on asymmetries in the surrounding charge. This type of very desirable bistable saturation suggests the possibility of quantum cellular automata arrays based on this type of cell.

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[8] Single electron cells have been discussed by P. Bakshi, D. A. Broido, and K. Kempa, J. Appl. Phys. **70**, 5150 (1991). The lack of the fundamental bistability in the response of a singly occupied cell makes their approach less promising.
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