Bistable saturation due to single electron charging in rings of tunnel junctions

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The behavior of rings of four small-capacitance tunnel junctions that are charged with two extra electrons is examined. Single electron charging effects result in quantization of charge on the metal electrode islands. To minimize the total electrostatic energy, the electrons localize on opposite electrodes, leading to a charge alignment in one of two configurations. We consider such rings as cells that may be capacitively coupled to each other in a cellular automaton architecture. The interaction between cells results in strong bistable saturation in the cell's charge alignment which may be used to encode binary information. Lines of such cells can be viewed as binary wires.

I. INTRODUCTION

Several schemes have been proposed for using Coulomb effects in small metal tunnel junctions to produce potentially useful behavior.[1,2] These have primarily exploited the Coulomb blockade of a tunneling current to produce single electron transistor action. The behavior of one- and two-dimensional arrays of small-capacitance tunnel junctions has also received considerable attention.[3]

Recently, we have theoretically examined the behavior of few-electron systems composed of quantum dots such as are usually fabricated in semiconductor heterostructures. We have shown bistable saturation in the charge alignment within quantum-dot cells that are Coulombically coupled to neighboring cells. This bistable interaction has formed the basis of a new architecture, termed quantum cellular automata (QCA).[4–7] Within the framework of this architecture, we have performed quantum simulations of designs for implementing binary wires, programmable logic gates, coplanar wire crossings, and circuits as complex as full adders.[8] The key advantages of the architecture are (1) only coupling between neighboring cells is necessary and this coupling is provided by the Coulomb interaction, (2) no power needs to be supplied to cells except at the edges of the array, (3) the design is robust in that it is insensitive to variations in physical parameters from cell to cell, and (4) as devices are reduced in dimension, the performance improves.

We examine here the behavior of cells composed of rings of metallic tunnel junctions with very small capacitance. The behavior of the rings is dominated by Coulomb exclusion effects.[9] We demonstrate that cells formed from these metal capacitors have the requisite bistable saturation and near-neighbor coupling behavior needed to provide the basis for an alternative implementation of the QCA architecture. The cell described here differs from those described elsewhere[4–8] in two fundamental ways. First, the cell is fabricated from small metal "islands" rather than from depleted two-dimensional electron gas and therefore contains many conduction electrons. Second, the coupling between islands and between cells is capacitive rather than simply Coulombic–the relevant Hamiltonian contains the capacitance matrix for the metallic array. This capacitive coupling is more amenable to control and design than the bare Coulomb interaction used in semiconductor implementation.

II. MODEL

We consider a cell consisting of four metal electrodes with small-capacitance tunnel junctions between them arranged in a ring, as shown schematically in Fig. 1(a). Each cell is occupied by two *extra* electrons supplied by the grounded substrate. The two electrons tend to occupy antipodal electrodes in the cell due to their mutual Coulomb repulsion.[10] This results in a preferential alignment of cell charge along one of the two perpendicular cell axes, as shown in Fig. 1(b). We define a polarization P which measures the extent of this alignment. If the charge on electrode i is ρ_i, then the polarization is defined as

$$P \equiv \frac{(\rho_1+\rho_3)-(\rho_2+\rho_4)}{\rho_1+\rho_2+\rho_3+\rho_4}. \quad (1)$$

If the extra electrons are completely localized on electrodes 1 and 3, the polarization is $+1$; if they are localized on electrodes 2 and 4, the polarization is -1. The presence of tunneling between electrodes means that the number of electrons on a metal electrode is not necessarily a good quantum number (it is a good quantum number in the limit of very little tunneling), so the ρ_i's need not be integers. Neighboring cells are capacitively coupled but no tunneling occurs between them.

The Hamiltonian[11] that describes the extra electrons in a cell labelled k can be written as follows:

$$H^k = \frac{1}{2} \sum_{i,j \in \text{cell } k} e^2 (\mathbf{C}^{-1})_{i,j} \hat{n}_i \hat{n}_j + \sum_{\substack{i \in \text{cell } k \\ j \notin \text{cell } k}} e^2 (\mathbf{C}^{-1})_{i,j} \hat{n}_i \hat{n}_j + \sum_{\substack{i,j \in \text{cell } k \\ i>j}} t_{i,j} (a_i^\dagger a_j + a_j^\dagger a_i). \quad (2)$$

Here $\mathbf{C}$ is the capacitance matrix describing the cell and the conductors surrounding it. The operators $a_i^\dagger$ and a_i create

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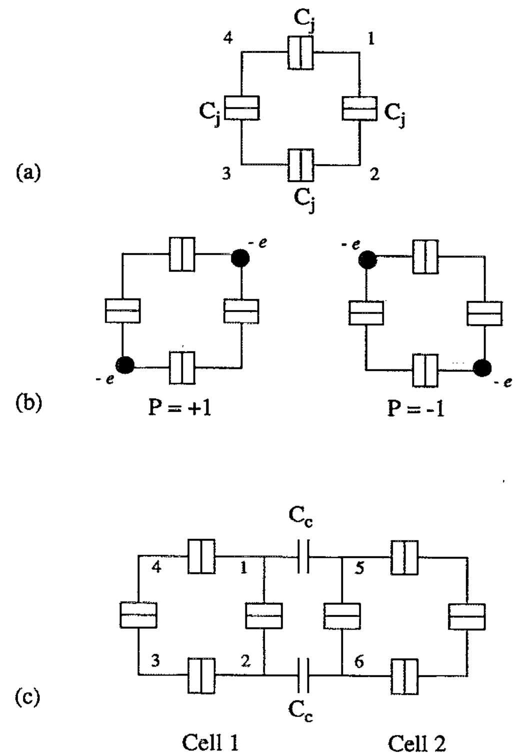

FIG. 1. (a) The ring of tunnel junctions that forms a basic cell. (b) Coulomb effects tend to localize the two extra electrons in one of the two configurations shown. These have polarization of +1 and −1. (c) Two capacitively coupled cells.

and annihilate, respectively, an extra electron on conductor i. The number operator $\hat{n}_i \equiv a_i^\dagger a_i$ counts the number of extra electrons. The first term in Eq. (2) represents the electrostatic energy due to the interaction of charges within the cell. The second term represents the energy of interaction between the conductors in the cell and the charges on neighboring conductors. The third term represents the tunneling of the extra electrons through the tunnel junctions between the conductors in the cell. The Coulombic effects in the first two terms tend to localize the electrons on antipodal electrodes. The tunneling term opposes this localization, a reflection of the kinetic cost of confinement. We take $t_{i,j}$ to be nonzero only between electrodes connected by a tunnel junction. All the tunnel junctions have the same tunneling energy t, which we express as a ratio to the charging energy of the junction[12]

$$t_{i,i+1} = t = \frac{\alpha e^2}{2C_j}. \tag{3}$$

The capacitance matrix **C** describes the capacitance of the four electrodes in the cell and the closest electrodes in each neighboring cell. For example, if the cell k has a neighboring cell to the right and left of it, **C** would include the nearest two electrodes in each cell. The size of **C** would therefore be 8×8. The capacitance to ground of each conductor is also included.

It is important to note that conductors in adjacent cells alter the cell Hamiltonian in two ways. First, they change the capacitance of the electrodes in the cell, thus altering the first term in the cell Hamiltonian (2) through changes in the capacitance matrix. The first term in this way includes the effect of the image charge induced on a (possibly uncharged) nearby conductor by the presence of charge in the cell. Second, if the nearby conductors are charged, they change the second term in the cell Hamiltonian which accounts for the Coulombic repulsion between an electron in the cell and one in a neighboring cell.

III. RESULTS

We examine the response of a cell to polarization, as just defined, of a neighboring cell. Consider a single cell, labeled cell 1, capacitively coupled to an adjoining cell, labeled cell 2, as shown in Fig. 1(c). The charge on electrodes 5 and 6 couples to the Hamiltonian for cell 1. We use values of the capacitances consistent with those experimentally determined for the structure described in Ref. 13. We take the tunnel junction capacitance $C_j = 600$ aF, the capacitance to the grounded substrate $C_g = 80$ aF, and the cell-cell coupling capacitance $C_c = 25$ aF. Note that all electrodes have the same shape and size and therefore the same capacitance to ground.

A charge of $(1-P_2)(-e/2)$ is placed on electrode 5, a charge of $(1+P_2)(-e/2)$ is placed on electrode 6, and the value of P_2 is varied from -1 to $+1$. (Because the remaining electrodes in cell 2 do not couple directly to cell 1, they play no role here.) For each value of the polarization P_2, we calculate the Hamiltonian for cell 1 and solve the corresponding Schrödinger equation. From the two-electron ground-state wave function, we calculate the charge on each site by calculating the expectation value of the (extra electron) number operator, $\rho_i = -e\langle \hat{n}_i \rangle$. The *induced* polarization of cell 1 can then be calculated using Eq. (1).

The polarization of cell 1 as a function of the polarization of the driver cell 2 we term the cell-cell response function; it is shown in Fig. 2 for $\alpha = 0.001$, 0.005, and 0.01. The highly nonlinear saturation of this function at both extremes of the polarization is key to the behavior of cellular arrays and makes the cells described promising candidates for cellular automata application. Even a rather slight polarization of a cell induces a nearly complete polarization of the neighboring cell. Because each cell in an array is essentially always polarized, the polarization of the cell can be used to encode binary information.

As α (and therefore t) increases, the response curve becomes less abrupt. Higher values of the tunneling energy t correspond to more tunneling. As tunneling increases, the (always approximate) requirement that the particle number in each electrode be quantized is relaxed. The electronic wave function distributes itself among the four electrodes in order to minimize the kinetic energy cost of confinement. For the QCA architecture to be effective, the particle number must be nearly quantized, so we require that the tunneling energy t be sufficiently small. This corresponds to the usual requirement that the resistance of the tunnel junctions be large compared to the quantum resis-

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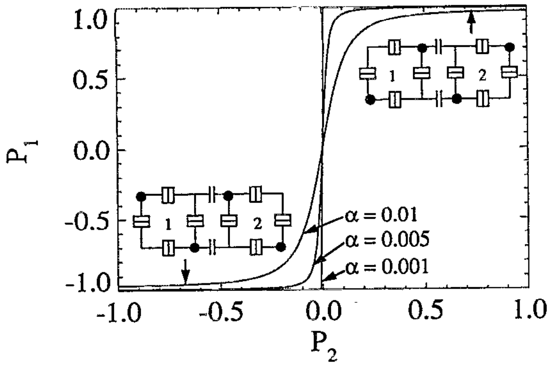

FIG. 2. The cell-cell response function for two capacitively coupled cells as shown in Fig. 1(c). The polarization of cell 2 is fixed and the induced polarization of cell 1 is calculated by solving the two-electron Schrödinger equation using the Hamiltonian (2). The strong bistable saturation of the induced polarization is the basis for *CA* behavior in these cells. Even a slight polarization of a cell induces a large polarization in a neighboring cell. The parameter α is the ratio of the tunneling matrix element to the charging energy of one capacitor. Small values of α correspond to less tunneling across the capacitor.

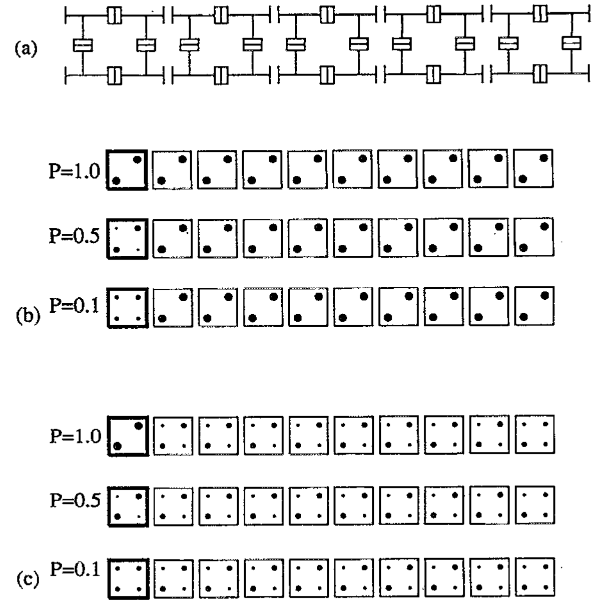

FIG. 3. Polarization of lines of capacitively coupled cells. (a) Schematic of a linear array of tunnel junction rings. (b) The calculated charge on each electrode in the array is shown for three different "driver" cell polarizations. The diameter of each filled circle is proportional to the charge on the corresponding electrode island. The results for small tunneling, corresponding to $\alpha=0.001$ are shown in (b) and the results for large tunneling, corresponding to $\alpha=0.05$, are shown in (c). If tunneling is too large, the requirement of charge quantization on each island is relaxed.

tance, $R_Q=h/(4e^2)$, for Coulomb blockade effects to be observable.[2]

We consider next a linear array of capacitively coupled cells. The Hamiltonian for an array of cells is simply the sum of the cell Hamiltonians, the coupling between cells being already explicit in (2). The wave functions for electrons in different cells do not overlap. We therefore use a direct-product basis composed of state vectors for each cell. We solve the time-independent Schrödinger equation for the ground state of the array in this basis using a Hartree-type self-consistent scheme, the intercellular Hartree approximation.[4] The Schrödinger equation is solved for each cell in the array, with the charges in all other cells kept fixed. The charges in each cell are then iteratively updated until convergence is obtained.

A linear array of coupled cells is depicted schematically in Fig. 3(a). The polarization of the first cell in the array is fixed. The charge on each of the electrodes in the remaining nine cells is calculated by self-consistently solving the Schrödinger equation for all cells in the array, as was previously described. The diameter of each of the dots in the figure is proportional to the charge on the corresponding electrode. Figure 3(b) displays the results when $\alpha=0.001$. The three driver polarizations shown, $P=1.0$, 0.5, and 0.1, are all quite successful at inducing complete polarization in the line of cells. The system is in this way "forgiving." Variations in parameters between cells may result in a given cell having a slightly lower polarization, but the response of the neighbors is so nonlinear that the polarization is quickly restored to its saturation value of nearly 1 (or -1). The nonlinear cell-cell response function plays the role of gain in conventional digital devices, restoring the signal level at each stage. The linear array of cells thus forms a binary wire capable of transmitting bit information encoded in the cell polarization.

For comparison, Fig. 3(c) displays the results of the wire response for the case where $\alpha=0.05$. In this case tunneling is strong enough to eliminate the quantization of charge on each electrode. The polarization nevertheless saturates at a value of $P=0.31$, regardless of the driver polarization. This case of strong tunneling, when the wire works rather poorly, serves to illustrate the mechanism through which it works well when tunneling is weak.

By directly solving the Hamiltonian system we have assumed that the electronic state of the four-metal islands in one cell form a quantum mechanical coherent system. If the cell is smaller than the phase-breaking length in the metal, this assumption is well-justified. If the cell is significantly larger, the treatment can be replaced by the semiclassical theory.[1] Since no current flows through the circuit, however, the semi-classical treatment amounts to finding the configuration of charges that minimizes the total electrostatic energy, subject to the constraint of charge quantization on each electrode. This is equivalent to neglecting the tunneling term in the cell Hamiltonian (2), and so corresponds to the small-t limit previously discussed and shown in Fig. 3(b).

Experimentally realizing cells of the type we discuss presents some challenges, but recent experiments indicate they are not insurmountable. Maintaining the double charging of each ring could be accomplished by using an insulated top gate, a conducting substrate to supply the electrons, and a thin tunnel barrier between the cells and the substrate to stabilize the charge at integer values. This method of controlling the charge state of ultrasmall structures has been demonstrated by Meuer *et al.*[14] and

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Ashori[15] in semiconductor quantum dots.[16] The problem of setting the polarization of a cell (writing the inputs) and sensing the polarization of a cell (reading the outputs) amounts to the problem of measuring the presence of individual electronic charges on a metal electrode. That this is feasible has been experimentally demonstrated by Lafarge and co-workers.[13] The analogous experiment using a semiconductor system has also recently been reported by Field *et al.*[17] As with all structures dependent on single-electron effects, those envisioned here would ultimately require that both variations in "polarization charges" resulting from variations in work functions and the presence of random trapped charges be rigorously controlled.

IV. CONCLUSIONS

We have shown that a cell composed of a ring of four metal electrodes connected by small-capacitance tunnel junctions exhibits bistable behavior when capacitively coupled to other similar cells. This behavior makes such cells candidates for realizing quantum cellular automata architectures.

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[9] Coulomb exclusion refers to a slightly different phenomenon than the usual Coulomb blockade of tunneling current. It denotes the exclusion of an electron from a region of space due to the Coulomb interaction with other electrons. See C. S. Lent, in *Nanostructures and Mesoscopic Systems*, edited by W. P. Kirk and M. A. Reed (Academic, Boston, 1992), p. 183; L. F. Register and K. Hess, *ibid.*, p. 369.

[10] A simple estimate of the electrostatic energy difference between the configuration with electrons on sites 1 and 2 and the configuration with electrons on sites 1 and 3 shows the latter to be lower in energy by $e^2/(8C_j)$.

[11] The use of a Hamiltonian and the coherent description employed here is strictly valid only at zero temperature when one can assume a unique ground state for each island. At nonzero temperatures, a manifold of nearly degenerate states becomes available for hopping into and irreversible processes must be included.

[12] The resistance of the junction is inversely related to the product of $|t|^2$ and the density of states at the Fermi energy. See A. A. Abrikosov, *Fundamentals of the Theory of Metals* (North-Holland, Amsterdam, 1988), p. 548.

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[16] One could alternatively supply electrons from another circuit in the plane of the cells and rely on the Coulomb blockade to stabilize the cell occupancy. This approach is used by the Saclay group in Ref. 13. Ultimately, we think the approach we outline will prove preferable because it does not require separate current-carrying contacts to each cell, a key advantage of quantum cellular automata architectures.

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