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Effect of Stray Charge on Quantum Cellular Automata

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We study the operation of quantum cellular automata (QCA) devices in the presence of stray charge. The operation of linear arrays of QCA cells, called binary wires, relies on Coulombic interaction between the cells, which is affected by the presence of such stray charge. The position of the charge determines whether or not the devices function properly, and it is possible to determine the "forbidden" region near the array in which the presence of stray charge causes device failure. We calculate this forbidden region by directly diagonalizing the Hamiltonian for the system including the stray charge. We find that the QCA binary wire is unaffected by stray charge at a distance greater than the intercellular repeat distance of the wire.

KEYWORDS: QCA, quantum cellular automata, stray charge, forbidden region, quantum dots

1. Introduction

We have proposed a new computer architecture called quantum cellular automata (QCA), in which two-electron quantum dot molecules serve as the cells of a cellular automata array.[1-6] A schematic of such a molecule, or cell, is shown in Fig. 1(a). The two electrons are allowed to tunnel between the five sites, but the interdot barriers are high enough that each electron is largely localized on a single quantum dot. The Hamiltonian used to describe this model cell is

$$H_0 = \sum_{i,\sigma} E_0 n_{i,\sigma} + \sum_{i>j,\sigma} t_{i,j}(a^\dagger_{i,\sigma} a_{j,\sigma} + a^\dagger_{j,\sigma} a_{i,\sigma}) + \sum_i E_Q n_{i,\uparrow} n_{i,\downarrow} + \sum_{i>j,\sigma,\sigma'} V_Q \frac{n_{i,\sigma} n_{j,\sigma'}}{\mid \boldsymbol{R}_i - \boldsymbol{R}_j \mid}. \quad (1)$$

The Coulombic interaction between the two electrons within a cell causes them to align in one of the two antipodal states shown schematically in Fig. 1(b). Interactions between nearby cells cause the state of the cell to switch between these two states in a very nonlinear manner. We call such behavior bistable saturation, since a very slight polarization of one cell can induce full polarization in neighboring cells. This behavior is analogous to gain in conventional digital devices, and allows the array to overcome local decreases in polarization.

Figure 2 shows two lines of such cells, each being driven by a cell of different polarization from the left end. It is important to note that Fig. 2 is not schematic; it shows the actual result of a calculation of the ground state of the system. The radius of each dot is proportional to the charge density located at that site. In Fig. 2(a), a line of cells, or "binary wire", is being driven from the left by a cell of polarization 0.8. This driver cell is almost completely polarized, and it drives the line so that the state of the cell on the right matches that of the driver cell. Thus the information contained in the state of the driver cell is transmitted to the other end of the binary wire. In Fig. 2(b), the wire is being driven by a very weakly polarized cell with $P = 0.02$. Even though this cell is weakly polarized, the bistable saturation behavior of the cells composing the line causes them to rapidly return to their fully polarized state. Thus, it is possible to recover from a local decrease in the polarization while transmitting information down a binary wire.

2. Effects of Stray Charge

Clearly, Coulombic interaction between cells of a binary wire is critical to the correct transmission of information. The presence of stray charges due to fabrication imperfections can cause such binary wires to fail, but total elimination of such charges may be difficult. We calculate the ground state of the electrons in a binary wire in the presence of a stray charge and determine in what situations the charge will cause the device to fail and in what situations the device will operate correctly despite the stray charge.

Figure 3 shows the result of many such calculations of the operation of a binary wire in the presence of a stray charge. The position of the stray charge is varied, and its sign and magnitude are identical to those of an electron. Due to the bistable saturation behavior of the cells composing the binary wire, the output of the wire is never indeterminate; it is always completely polarized

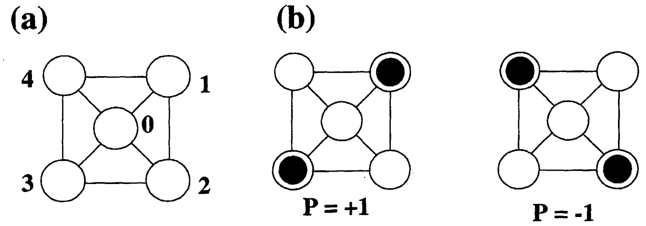

Fig. 1. A model QCA cell. (a) A schematic of the model cell. Two electrons tunnel between the five sites of each cell. (b) The two polarization states. The Coulombic interaction between electrons causes the cell to align in one of the two states shown, indicated by $P = +1$ and $P = -1$.

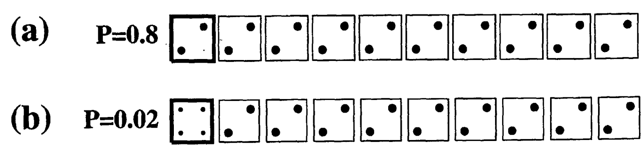

Fig. 2. Binary wires. (a) The information in the fixed driver cell (with the darker border) is transmitted to the other end of the wire. (b) Bistable saturation allows the weakly polarized cell to drive the wire to full polarization.

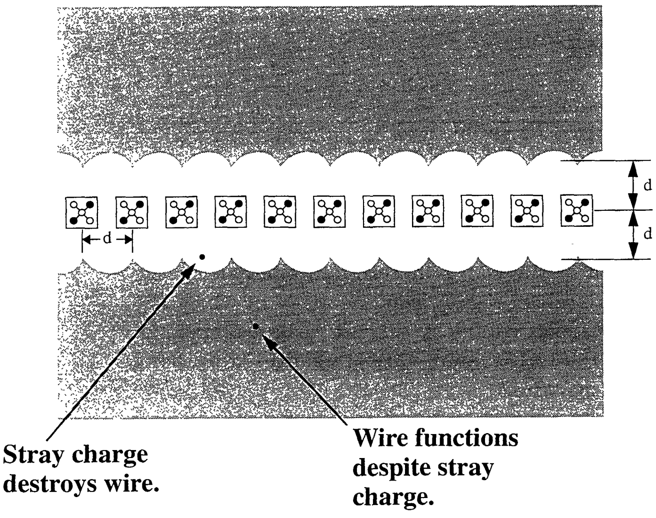

Fig. 3. Effect of stray charge on a single binary wire. An electron in the forbidden white region surrounding the wire will cause the system to fail, but the system will operate correctly in the presence of an electron in the shaded region. While the cells are schematic, the shape of the transition is the result of many actual binary wire simulations.

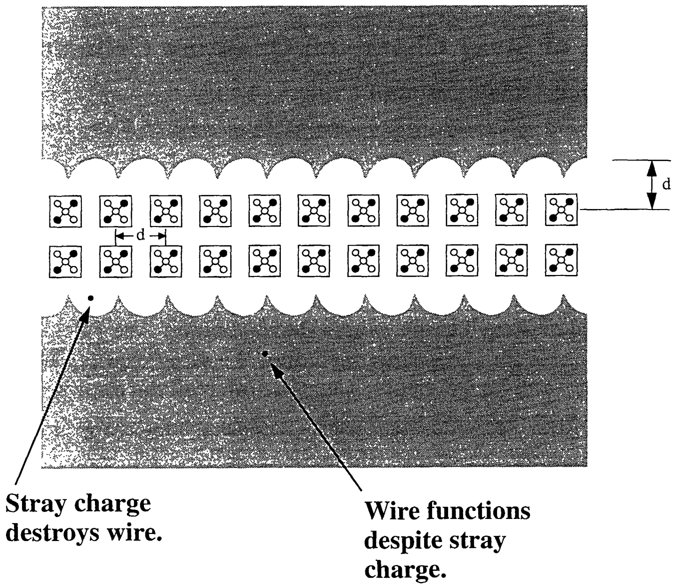

Fig. 4. Effect of stray charge on a double binary wire. The forbidden region on each side of the wire is smaller for this more reliable device, but the area required for the second wire actually increases the size of the forbidden region.

in one of the two directions. Depending on its agreement or disagreement with the driver cell, the wire can be said to have completely worked or completely failed.

The border between these two outcomes is very sharp; moving the stray charge by less than a nanometer can cause the outcome to change. Thus, the area around the device can be divided into two parts: the region in which the stray charge causes the device to fail (the "forbidden" region) and that in which the device works properly despite the stray charge (the "allowed" region). Determination of the border between these two regions requires many simulations of the binary wire with the stray charge located at various positions. For each position, we consider both driver inputs, polarizations $+1$ and -1, and check for failure of the wire to transmit this input.

Because of the Coulombic nature of the interaction between the binary wire and the stray charge, the strength of the interaction depends on the distance from the wire to the stray charge. When the charge is very close to the wire, its effect is great, and it always causes the wire to fail. As the stray charge is moved away from the wire, the Coulombic interaction decreases until the effect of the stray charge on the wire is completely negligible. In between these two extremes is the transition point at which the stray charge is far enough away from the wire that it just barely operates correctly. There is a single such transition distance from the wire for any given horizontal position along the wire. Determination of a series of these transition points for many horizontal positions allows us to determine the shape of the border between the forbidden region and the allowed region.

We determine each transition point by successively refining an upper and a lower bound within which the border point is contained. The upper point is always in the allowed region, while the lower point is kept in the forbidden region. The point midway between the two is simulated, and replaces either the upper or lower point depending on whether the binary wire succeeded or failed. Thus, the uncertainty in the position of the transition point is halved with each new simulation. In theory, this could determine the position of the transition to any precision, but we perform the calculation to a tolerance of approximately one-tenth of a nanometer. Each simulation involves finding the ground state of the system by directly diagonalizing the Hamiltonian for the entire wire in the presence of the stray charge.

Repetition of this calculation for a series of horizontal positions gives a series of transition points and traces out the two-dimensional region in which a stray charge will cause the wire to fail. Since the simulated wire is sufficiently long that edge effects are negligible near the middle of the wire, the environment of a given cell is almost identical to that of its neighbors. Therefore, the pattern of the border between the two regions repeats itself with each cell. It is only necessary, therefore, to perform the calculation throughout a unit cell near the middle of the array.

For this reason, the cells in Fig. 3 are shown schematically to indicate that the periodic nature of the border is due to the fact that the simulated wire is considered to continue infinitely in both directions. It is important to note that although the cells in Fig. 3 are schematic, the shape of the border is the result of the actual calculation described above. The cells are drawn to scale with the forbidden region, which is approximately as wide as the intercellular spacing. The inward curve of the forbidden region near the center of each cell is due to the symmetry of the cells composing the wire; the effect of stray charge is less when it is near the horizontal center of a cell, so the allowed region is closer to the wire at those positions.

Figure 4 shows a similar calculation for a "double binary wire". In this case, two parallel binary wires are placed close enough together that each reinforces the information carried by the other. Introducing an error in such a wire requires twice as much energy as introducing an error in a single binary wire, so such double wires have higher reliability than single wires. The same procedure was followed to determine the border between the allowed region and the forbidden region in this case, and the results show that the stray charge can come closer to either side of the double wire than it could come to the single wire. However, the extra width of the forbidden region introduced by the presence of the second wire more than offsets this gain. We conclude that while double wires may be more reliable than single wires, they provide no extra insurance against errors due to stray charges. In fact, a double wire produces a slightly larger area in which a stray charge causes failure of the wire.

3. Conclusions

The effect of stray charge on single and double binary wires has been studied. We have found that the transition between the allowed region and the forbidden region for stray charge is very sharp, and it occurs approximately one intercellular distance away from the wire. This distance is slightly less for a double binary wire, but the improvement is offset by the extra space required for the second parallel wire.

Acknowledgements

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