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A new phenomenon of quantum-dot cellular automata

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Abstract: If an external point charge and the movable charges of an isolated quantum-dot cellular automata (QCA) cell have the same polarity, the point charge greatly affects the polarization (P) of the cell only when it is in a narrow band with periodically changing width. The center of the band is on a radius R circle. The ratio of R to the electric charge (q) is a constant determined by the parameters of the cell. A QCA cell can be used as charge detector based on the above phenomenon.

Key words: Quantum-dot cellular automata (QCA), Quantum dot, Hubbard-type Hamiltonian
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INTRODUCTION

The concept of logic circuits based on quantum-dot cellular automata (QCA) has received much attention since it was first proposed by Lent *et al*. (1993) due to prospects of extremely low-power operation and drastic reduction of interconnections. The basic QCA building block is represented by a bistable cell made up of four quantum dots or metallic islands at the vertices of a square and containing two electrons that can align along two different diagonals, thus encoding two logical states. An isolated cell, alignment along either diagonal is equally likely, but in the presence of a driver cell whose polarization along one of the diagonals is externally enforced, the electrons in the driver cell will align along the same diagonal, so that the total electrostatic energy is minimized. It is therefore possible to propagate the polarization state along a chain of cells.

Much work (Tougaw and Lent, 1994; Gin *et al*., 1999) has been done on the cell-cell interaction with the results showing that all combinatorial logic circuits can be realized with QCA cells. In addition to the logic circuits being used for arithmetic and logic operation, the cells can be deliberately arranged to realize application-specific circuits (Pasky *et al*., 2000). All such circuits use the high non-linearity of cell-cell interaction. Study (Toth and Lent, 1999; Bonci *et al*., 2002) on the dynamical behavior of QCA circuits indicated that the circuits should work adiabatically by clocked switching for two main reasons. One is that the adiabatic switching can ensure the circuits work correctly, and the other is that the speed of the circuits can be controlled. Moreover, a merit of the clocked switching method is that it makes the cells' storage of information much easier. Various implementations (Orlov *et al*., 1998; 1997; Amlani *et al*., 1999) of QCA cell based on metal islands, on quantum dots obtained in semiconductor heterostructures, or on nano-structured silicon islands have been proposed so far. For the purpose of room temperature work, the cells must be very small, so small and uniform size candidate molecules have attracted intense attention (Lent and Isaksen, 2003; Collier *et al*., 1999) recently. Bad effects resulted from imperfections, temperature and stray charge had also been studied (Yakimenko *et al*., 1999; Ungarelli *et al*., 2000; Tougaw and Lent, 1995).

There were investigations on effect of stray charge on QCA circuits. However, stray charge may produce different effect on an isolated QCA cell since it is different from QCA circuits. The effect of an

external point charge on an isolated QCA cell has not been reported by far. Our work on stray charge yielded many interesting results.

SIMULATION METHOD

We used a cell made up of four quantum dots at the vertices of a square and containing two excess electrons, as schematically shown in Fig.1. Polarization (P) is used to characterize the cell and can be written as follows:

$$P=\frac{\rho_1+\rho_3-\rho_2-\rho_4}{\rho_1+\rho_2+\rho_3+\rho_4} \tag{1}$$

where ρ_i denotes the electron probability density at dot i. To maintain charge neutrality, a fixed +0.5e (e is electron charge) charge is assumed at each dot. A tight-binding Hubbard-type Hamiltonian was used to model the quantum cell. Ignoring any degrees of freedom internal to the dots, the Hamiltonian for a single cell can be written as:

$$H^{\text{cell}}=\sum_{i,\sigma}(E_0+V_i)\hat{n}_{i,\sigma}+\sum_{i>j,\sigma}t_{i,j}(\hat{a}_{i,\sigma}\hat{a}_{j,\sigma}+\hat{a}_{j,\sigma}\hat{a}_{i,\sigma})+\sum_i E_Q\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}+\sum_{i>j,\sigma,\sigma'}V_Q\frac{\hat{n}_{i,\sigma}\hat{n}_{j,\sigma'}}{|\boldsymbol{R}_i-\boldsymbol{R}_j|} \tag{2}$$

where $\hat{a}_{i,\sigma}$ is the annihilation operator that destroys a particle at dot i with spin σ, the number operator for dot i and spin σ is represented by $\hat{n}_{i,j}$, E_0 is the on-site energy for each dot, V_i is the energy on dot i due to effects from external charges, $t_{i,j}$ is the energy associated with tunneling between dots i and j, and E_Q is the on-site charging energy (the purely Coulombic cost for two electrons of opposite spin to occupy the same dot). The last term represents the Coulombic potential energy for two electrons located on dots i and j. V_Q is an electrostatic parameter fixed by fundamental constants and the dielectric constant of the material used to form the cell.

The spins of the two electrons in the cell can be either parallel or antiparallel. We consider here the case of electrons with antiparallel spins, since that is the ground state of the cell. Calculations with electrons having parallel spins yield qualitatively very similar results. In our system, V_i is produced by the external point charge, so it can be written as:

$$V_i=V_Q\frac{q}{|\boldsymbol{R}_q-\boldsymbol{R}_i|} \tag{3}$$

where q is the electric charge and $\boldsymbol{R}_q$ is the position of the charge. For the steady-state problem, the following time-independent Schrödinger equation is used,

$$H^{\text{cell}}|\Psi_i\rangle=E_i|\Psi_i\rangle \tag{4}$$

where $|\Psi_i\rangle$ is ith eigenstate of the Hamiltonian, and E_i is the corresponding eigenvalue. From Eq.(4) we can get the ground state of the cell and then P can be calculated.

As the parameters of the cell, we take E_0 to be zero, the distance between two neighboring dots (a) 20 nm, and the diameter of quantum dot (D) 10 nm. The coulomb coupling strength (V_Q) is calculated for a material with a dielectric constant of 10 and its value is 143.8 meV, and E_Q is taken to be $V_Q/(D/3)$. The tunneling energy between neighboring dots is t=0.3 meV and 0 for antipodal dots.

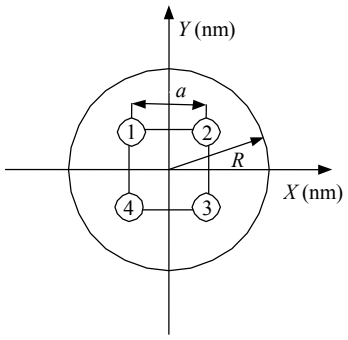
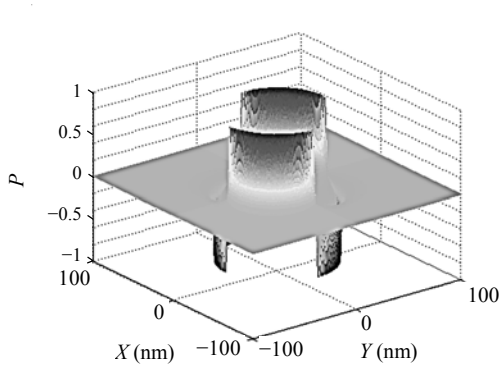


Fig.1 The cell and the coordinates

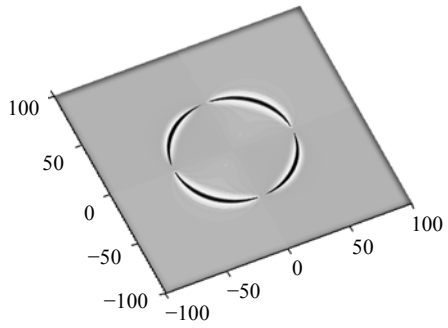
RESULT

We investigated how P is influenced by an external point charge on the X-Y plane. As shown in Fig.2, a –0.3e point charge greatly affects P only when it is in a narrow band with periodically changing width. The center of the band is on a radius R circle. The figure indicates that the response of P to the charge dependent strongly on the positions of the charge. The reciprocal of the bandwidth can be used

to represent the degree of dependence, which minimizes when the charge aligns in direction of the cell diagonals and maximizes when the charge aligns in the direction of the X or Y axis. The dependence degree decreases as t decreases. For example, the dependence degree decreases by 10 percent when t changes from 0.3 to 0.2 meV for the system described above. The dependence degree and the largest P can be seen more clearly from Fig.3.



(a)



(b)

Fig.2 (a) P vs the position of a −0.3e point charge on X-Y plane; (b) The top view of (a)

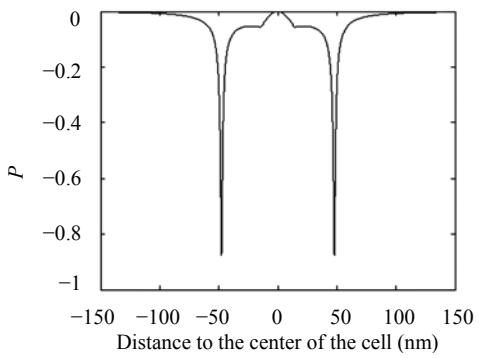


Fig.3 P vs the position of a –0.3e point charge on the line through dots 1 and 3

Fixing the parameters of the cell, we checked the influence of the value of q on R and found that R changes linearly with q. So we define a new parameter K as

$$K=R/q \tag{5}$$

The value of K is determined only by the parameters of a cell. K is 159.2 (nm/e) for the cell described above. Compared to the dielectric constant of material, the relations of K to t and a are nonlinear. For the dielectric constant we used here, K is described by the following empirical Eq.(6).

$$K = 12 + 411.35\mathrm{e}^{(-t/0.1943)} + 3.77968a - 0.03948a^2 \tag{6}$$

If other dielectric constants are used instead, the above equation is still valid, only the constant term needs to be changed. From Eq.(6), we can see that K increases as t decreases.

In the above research, the point charge is negative and the cell has two excess electrons. We also calculated P for positive point charge. Fig.4 shows that P increases monotonically as an external positive charge approaches the cell. It should be pointed out that if the movable charges of the cell are positive, an external positive charge can produces the unusual phenomenon shown in Fig.2 while a negative charge will give a similar result as presented in Fig.4.

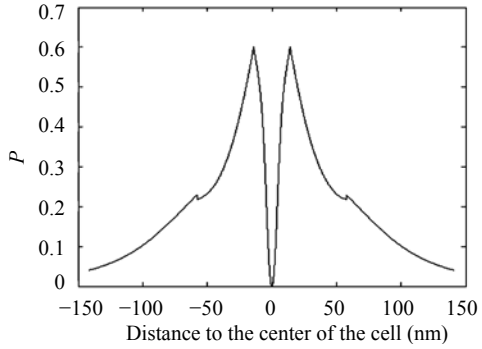


Fig.4 P vs the position of a +0.3e point charge on the line through dots 1 and 3

Fig.2b shows that P is very small when the charge is on X or Y axis. To verify the intuition, we studied the relation of P to the position of a –0.3e charge on X or Y axis and found that the peaks in Fig.5 have values almost equal to zero, so we can say that

the charge does not affect P. The result is independent of the polarity and value of the point charge.

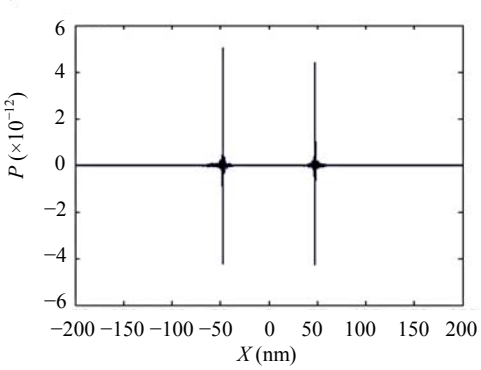


Fig.5 P vs the position of a –0.3e point charge on X axis

DISCUSSION

We think the above phenomenon has relation with the interaction energy (E_{inter}) between the charge and the cell and investigated the relation. As shown in Fig.6, on the whole the energy increases monotonically as the external charge approaches the cell if the charge is negative. However, there is a minimum inflexion point M whose position is on the circle illustrated in Fig.2b. It is the abrupt change of distribution of cell electrons that lowers the energy at position M. Thus, the polarization of the cell when the charge is on M is very different from the polarization of the cell when the charge is on M's neighbors. If the charge is positive, there is no inflexion point as illustrated in Fig.7.

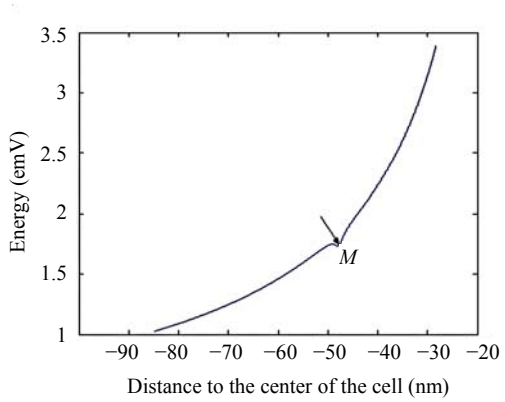


Fig.6 The interaction energy between the cell and a –0.3e point charge on the line through dots 1 and 3

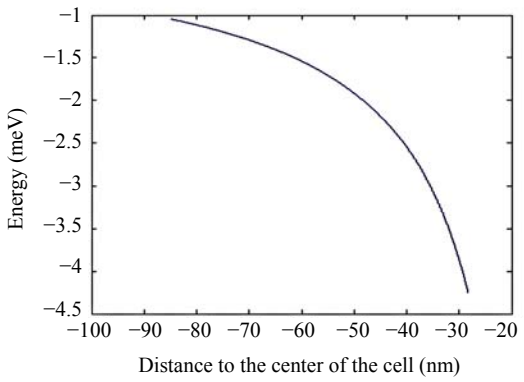


Fig.7 The interaction energy between the cell and a +0.3e point charge on the line through dots 1 and 3

Increasing t means that electrons of the cell have stronger dislocation trend, so larger E_{inter} is needed to produce the same effect on the cell. The position of M moves to the cell as t increases. Such relation is expressed in Eq.(6). When a becomes larger, the energy difference between two electrons on the diagonal and on the edge becomes smaller, which makes smaller E_{inter} capable of producing the same effect on P.

When a negative external charge is close to one dot of the cell, P is small too. We use an example to give a simple explanation. For example, when the negative charge is very close to dot 1, electrons have large probability to appear on dot 3 since it has the largest distance to dot 1. According to Eq.(1), P is still small although electrons hardly appear on dot 1. If the charge is positive, electrons have large probability to appear on dot 1 and some probability to appear on dot 3 because electron on dot 1 has strong repulsion force against other electrons as the electron on dot 1 is close to the external charge. Thus P is not near zero when the charge is close to dot 1.

CONCLUSION

We reported here a new phenomenon of quantum-dot cellular automata. A QCA cell can be used as charge detector based on the above phenomenon. If q is known, then the cell can detect the distance of the charge, and vice versa.

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