DYNAMIC BEHAVIOR OF COUPLED QUANTUM DOT CELLS*

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ABSTRACT

We examine the dynamic behavior of a large group of coupled quantum dots responding to a changing electrostatic environment. The electrons occupying the quantum dots interact Coulombically and tunnel between neighboring dots. To model this system, we solve the time-dependent Schrödinger equation over finite and semi-infinite domains. These ideas are used to model the dynamic behavior of binary wires, the most fundamental elements of quantum cellular automata. The results of these simulations highlight the importance of kink propagation at polarization domain interfaces.

I. INTRODUCTION

The use of quantum mechanics to design and model computational elements has given rise to several new paradigms for computation. Among these is computing with the ground state, in which the time-independent behavior of a system can be used to perform useful logical functions. When an input is applied to such a system, it changes the boundary conditions of the quantum state so that the system is no longer in the ground state. Unavoidable dissipation then drives the system into the ground state corresponding to the new input. Mapping inputs to outputs enables one to perform useful computation using the dissipation inherent in the array. Since the devices use the ground state to perform calculations, a great deal of design work can be done without regard to the dynamic behavior of the devices. It is possible that some devices will be unable to reach the ground state due to the presence of metastable states, but such states should be quite rare. Information about response time and the possible existence of metastable states requires time-dependent modeling of the system. Such dynamic modeling is the topic of this research.

One example of a system that uses computing with the ground state, quantum cellular automata, is explained in section II. This is followed in section III by a description of the energy-absorbing boundary conditions recently introduced by Hellums and Frensley. Section IV presents results showing the dynamic behavior of two different binary wires. Finally, section V presents conclusions and areas for further work.

II. QUANTUM CELLULAR AUTOMATA

One new scheme that takes advantage of computing with the ground state is called quantum cellular automata, or QCA [1-3]. As shown in figure 1, the cells that compose a QCA consist of four quantum dots where tunneling is allowed between neighbors and with two electrons shared among the four dots. The model Hamiltonian for this system is:

$$H = \sum_{i,\sigma} E_{0,i}\, n_{i,\sigma} - \sum_{i>j,\sigma} t_{i,j}\left(a_{i,\sigma}^{\dagger} a_{j,\sigma} + a_{j,\sigma}^{\dagger} a_{i,\sigma}\right) + \sum_{i>j,\sigma,\sigma'} V_Q \frac{n_{i,\sigma} n_{j,\sigma'}}{\left|\vec{R}_i - \vec{R}_j\right|} + \sum_{k\neq m,j} V_Q \frac{\left(n_{k,j} - \tilde{\rho}\right)}{\left|\vec{R}_{k,j} - \vec{R}_{m,i}\right|} \qquad (1)$$

This Hamiltonian contains second-quantized terms including on-site energies, tunneling between neighbors, and intracellular and intercellular Coulombic repulsion. Due to this repulsion between the two electrons, the charge density of the ground state of the cell is almost completely aligned in one of the two polarization states shown in figure 2. We can use this bistable saturation behavior to encode one bit of binary information in the quantum state of the cell.

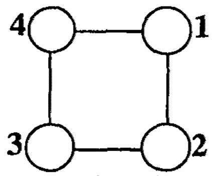

Figure 1. Schematic of a QCA cell. Two electrons are shared among the four sites, and tunneling is allowed between neighbors.

Figure 2. Antipodal alignment of electrons due to Coulombic repulsion.The ground state is highly bistable.

Figure 3 shows an arrangement of cells referred to as a binary wire [4]. In this arrangement, the polarization of each cell causes its neighbors to align in a similar direction, and the polarization information contained in the cell at one end of the wire is transmitted to the other end. The binary wire will be used to transmit polarization information from point to point in our scheme.

Figure 4 shows a group of cells which act as a majority logic gate. The cells on the top, bottom, and left sides have fixed polarizations, while the center cell and the output cell on the right are free to react to the polarizations of the other cells. When such a system is simulated, we find that the polarization of the free cells always aligns in the direction of a majority of the driving neighbors. Therefore, such an arrangement of cells performs majority logic on the three inputs.

If one of the three inputs is defined to be a program line, the device can be thought of as a programmable AND-OR gate. For example, if one of the inputs is held in the logical one state, the output of the majority device will also be one unless both of the other inputs are zero. The device therefore performs the OR operation on the two non-program inputs. Likewise, a zero on the program line causes the device to perform AND logic on the two non-program inputs.

Similar arrangements of QCA cells have been designed to perform inversion of a signal, coplanar crossing of wires, and dedicated AND and OR gates. Combinations of these devices have been used to synthesize more complex devices including exclusive-OR gates and full adders [5].

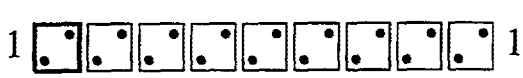

Figure 3. A binary wire. Dot radius on each site is proportional to the actual calculated charge density on that site. Data is transmitted from one end of the wire to the other.

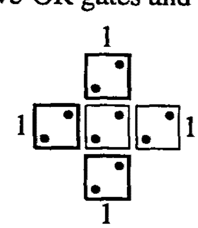

Figure 4. Majority logic gate. The state of the two free cells matches that of a majority of the driving cells.

III. ENERGY-ABSORBING BOUNDARY CONDITIONS

We model dissipation of kink energy in our system by the presence of a semi-infinite line of similar cells which can absorb kink energy. In this case, the time-dependent Schrödinger equation for the entire system (QCA device and reservoir) can be written as [6]:

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\Psi_s\\ \Psi_r\end{bmatrix} = \begin{bmatrix}H_s & H_i^{\dagger}\\ H_i & H_r\end{bmatrix}\begin{bmatrix}\Psi_s\\ \Psi_r\end{bmatrix} \tag{2}$$

where H_s is the Hamiltonian of the system given in equation (1), H_r is the Hamiltonian of the reservoir, and H_i is the interaction Hamiltonian between the two. As demonstrated recently by Hellums and Frensley, the effect of H_r is included by using the Green function of a semi-infinite line, which is well known. H_i introduces a time-dependent convolution integral over the past history of the system, which makes the equation non-separable and causes the boundary condition to be non-Markovian.

These non-Markovian boundary conditions cause the dynamics of the QCA device to be irreversible, even though the dynamics of the combined system are reversible. Proper impedance matching of the system-reservoir interaction will prevent kink reflections at the system-reservoir interface, while poor impedance matching can increase the relaxation time for kinks to leave the system.

IV. KINK PROPAGATION IN THE BINARY WIRE

When these ideas are applied to the binary wire shown in figure 3, we can demonstrate the dynamic response of a kink traveling from end of the wire to the other. Figure 5 shows the dynamic response of a wire with relatively low tunneling barriers, while figure 6 shows the response of a wire with higher barriers. At t=0, the polarization of the cell at the left end of the wire is switched and held constant. This introduces a kink in the polarization profile of the wire and places the system in an excited state. The kink propagates away from the fixed end and eventually leaves the wire through the open boundary condition. This dynamic analysis shows that the response time of the faster wire is approximately 30 ps, that of the slower wire is approximately 150 ps, and there are no metastable states to prevent the systems from returning to the ground state. Higher tunneling barriers cause slower relaxation but more highly polarized cells, while lower barriers give a faster relaxation time with more weakly polarized cells.

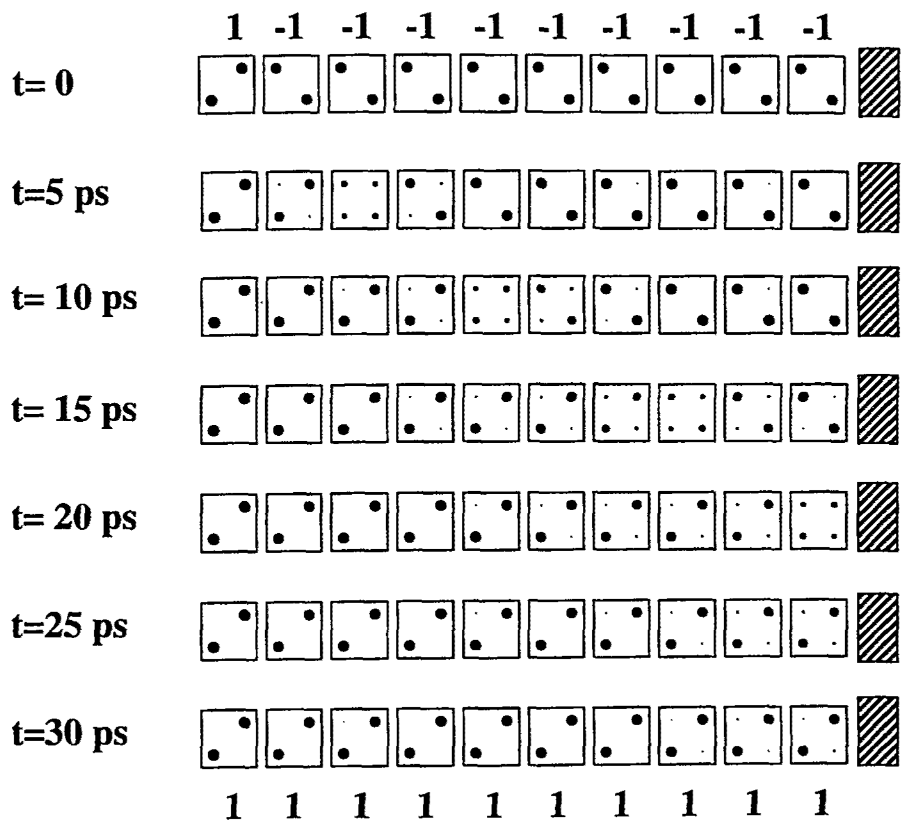

Figure 5. Kink propagation in a binary wire with a semi-infinite reservoir at the right end. These charge density plots show the state of the wire at different time steps. At t=0, a kink is introduced by flipping the left-most cell, and this kink has propagated out of the system into the semi-infinite reservoir by t=30 ps. Here, the tunneling coefficient is 3 meV, indicating relatively low tunneling barriers.

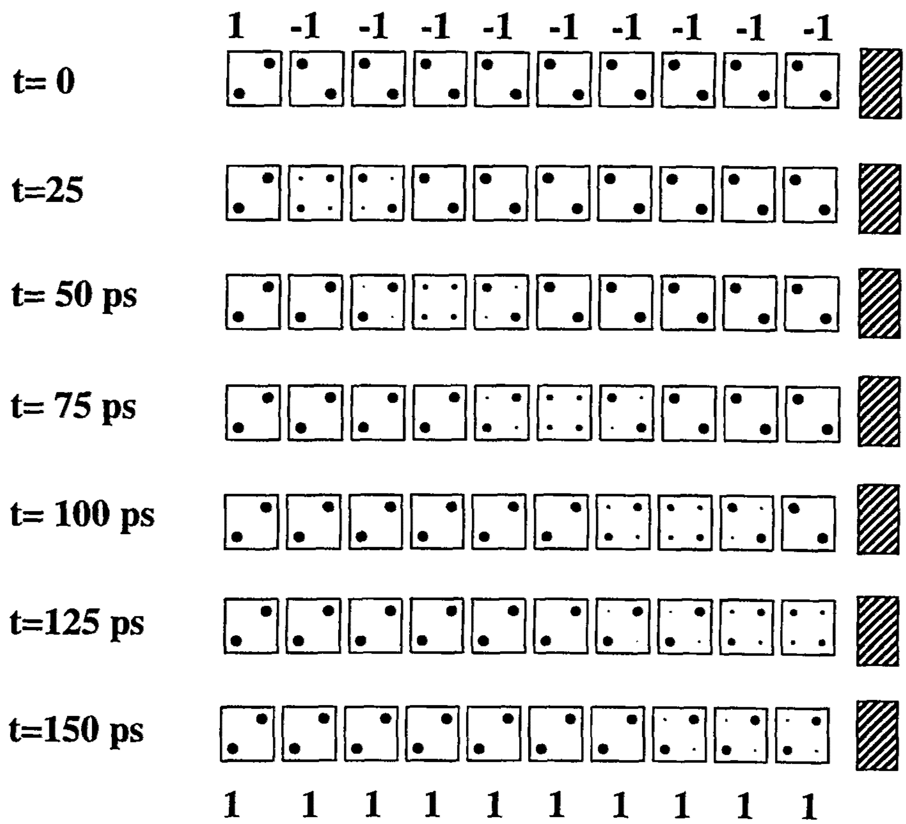

Figure 6. Kink propagation in a binary wire. The tunneling coefficient of this wire is 1.1 meV, indicating relatively high tunneling barriers. The response time of the wire is 150 ps, but the slower response time is accompanied by more highly polarized cells.

V. CONCLUSIONS

The introduction of open boundary conditions to the time-dependent model of QCA devices has allowed us to model the relaxation of the devices to their ground state. This dynamic analysis has provided useful information about relaxation times, as well as demonstrating the absence of metastable states. The importance of kink propagation in the relaxation of the binary wire was demonstrated.

Future directions for this research include more realistic models of dissipation throughout the system, dynamic modeling of more complex devices, and investigation of the impact of finite temperatures on device dynamics.

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1. C. S. Lent, P. D. Tougaw, and W. Porod, *Appl. Phys. Lett.* **62**, 714 (1993).
2. C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, *Nanotechnology* **4**, 49 (1993).
3. P. D. Tougaw, C. S. Lent, and W. Porod, *J. Appl. Phys.* **74**, 3558 (1993).
4. C. S. Lent and P. D. Tougaw, *J. Appl. Phys.* **74**, 6227 (1993).
5. P. D. Tougaw, C. S. Lent, and W. Porod, *J. Appl. Phys.* **75**,1818 (1994).
6. J. R. Hellums and W. R. Frensley, Phys. Rev. B **49**, 2904 (1994).