Quantum Computing with Quantum-dot Cellular Automata using Coherence Vector Formalism

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A coherence vector formalism is used to describe quantum computing with Quantum-dot Cellular Automata, and the realizations of basic quantum gates are also discussed.

1. Introduction

A nanoelectronics technology that would enable device scaling down to molecular levels will almost certainly entail a cellular architecture with near-neighbor connectivity. One scheme that has been developed for physically realizing such a concept is termed Quantum-dot Cellular Automata (QCA) [1-8] The basic cell is comprised of four or five dots which can hold two extra electrons. Information is encoded in the geometrical charge configuration within the cell. The Coulomb interaction between cells provides the inter-cellular coupling. This interaction produces a sufficiently rich system that it has been shown that could be implemented in such a scheme.

The two basis states of the QCA cell with polarization P=+1 and P=-1, respectively, are shown in Fig. 1.

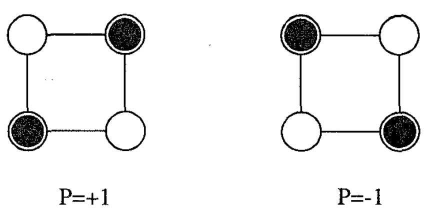

FIGURE 1. Schematic representation of the QCA cells. Two electrons tunnel between the four dots in the cell. The two arrangements of charge shown are used to encode information in the cell.

The empty circles denote a quantum dot, the lines show the possibility of interdot tunneling, and the solid circles indicate extra electron. Logical circuits (AND, OR, NOT gates) and Cellular Nonlinear Network [7,9-11] architectures can be both realized by this paradigm.

In this paper the so-called coherence vector formalism [12] will be applied to the QCA. Its main advantages are the mathematical simplicity and the ability of this description to include dissipation.

In Section 2 the physical background will be summarized, while Section 3 and 4 are about the realization of the Quantum Computing with QCA. Three basic operations will be implemented: the NOT, the controlled NOT and a three-bit quantum gate, that will be called modified *controlled controlled* NOT (MCCNOT) in this paper.

2. Application of the coherence vector formalism for QCA

The Hamiltonian of a single QCA cell of a 1D array is [7]:

$$H(\gamma) = \begin{bmatrix} E_0 - \frac{E_k \bar{P}}{2} & -\gamma \\ -\gamma & E_0 + \frac{E_k \bar{P}}{2} \end{bmatrix}$$

where γ is the interdot tunneling energy and E_k is the electrostatic cost of two adjacent fully polarized cells having opposite polarization. The cell is coupled to its left and right neighbors through $\bar{P}$ which is the sum of the adjacent cell polarizations.

The state vector of one cell can be given as the linear combination of the fully polarized P=+1 and P=-1 basis states.

$$|\Psi\rangle = \alpha|1\rangle + \beta|-1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

Thus the state of a cell is described by two complex numbers, α and β.

An alternative quantum mechanical description to the state vector is the $\vec{\lambda}$ *coherence vector.* For a two-state system its three real coordinates are the expectation values of the $\hat{\sigma}_x$, $\hat{\sigma}_y$ and $\hat{\sigma}_z$ Pauli spin matrices. The fully polarized P=+1 state corresponds to $\vec{\lambda}$=(0,0,-1) and the P=-1 state corresponds to $\vec{\lambda}$=(0,0,+1). The third coordinate of $\vec{\lambda}$ equals -P. The coherence vector description is used in this paper because it is more straightforward to design and interpret quantum computer operations and may make inclusion of dissipation effects possible.

For a non-dissipative system the dynamical equation of the coherence vector is[12]:

$$\frac{d\vec{\lambda}}{dt} = \vec{\Gamma} \times \vec{\lambda} \tag{1}$$

where the cross denotes vector product and $\vec{\Gamma} = Tr(\vec{\sigma}\hat{H})$ for the QCA cell is:

$$\hbar\vec{\Gamma} = \begin{bmatrix} -2\gamma \\ 0 \\ E_k\bar{P} \end{bmatrix}$$

This equation describes the precession of the coherence vector around $\vec{\Gamma}$. If there is no dissipation the length of the coherence vectors remains unity.

In the case of dissipation additional terms are required [13]:

$$\frac{d\vec{\lambda}}{dt} = \vec{\Gamma} \times \vec{\lambda} - \frac{1}{\tau}\left(\frac{1}{\tanh\Delta}\vec{\lambda} + \hat{\Gamma}\right) \tag{2}$$

Here τ is energy relaxation time, Δ is the temperature ratio:

$$\Delta = \frac{\hbar|\vec{\Gamma}|}{2k_B T}$$

and

$$\hat{\Gamma} = \frac{\vec{\Gamma}}{|\vec{\Gamma}|}$$

In (2) the first new term denotes the dissipation to the environment, the second one corresponds to the thermal fluctuation caused by the environment.

The steady state energy of a cell can be shown to be:

$$E_{ss} = -\frac{\hbar|\vec{\Gamma}|}{2}\tanh\Delta$$

The coherence vector of a cell in steady state is:

$$\vec{\lambda}_{ss} = -\hat{\Gamma}\tanh\Delta$$

As temperature increases *tanh* Δ decreases and the cell keeps loosing its polarization due to the effect of the fluctuation of the heat bath.

3. Quantum computing with QCA

In this section it is shown how to use a 1D array of QCA cells for quantum computing [14-26; for review see 14-15]. The NOT, controlled NOT and the MCCNOT operations will be realized by applying the coherence vector formalism and treating the intercellular interactions in a Hartree-Fock model. We omit dissipation effects in the present work.

The $\vec{\Gamma}$ vector will be used to manipulate the coherence vector. The Γ_x can be set externally by changing the interdot barrier height. The two extreme cases are: $\gamma=\infty$ (or from an implementation perspective $\gamma \gg E_k$) and $\gamma=0$.

In the first case $\hbar\vec{\Gamma}$=(-2γ,0,0) which causes λ to precess around the *-x* axis. This can be used to go from the $\vec{\lambda}$=(0,0,+1) state to the (0,0,-1) state and vica versa, realizing the NOT operation. We need 180° rotation thus the duration is $T=\pi/|\vec{\Gamma}|=\pi\hbar/2\gamma$. The operation of the NOT is shown in Fig. 2.

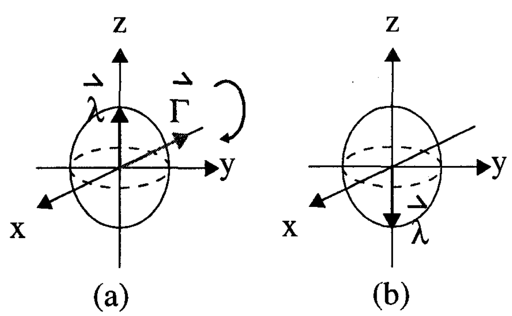

FIGURE 2. NOT operation. (a) The initial state is $\vec{\lambda}$=(0,0,+1) or P=-1. (b) The final state obtained after 180° rotation around the *x* axis in the negative direction is $\vec{\lambda}$=(0,0,-1) or P=+1.

In the second case $\hbar\vec{\Gamma}=(0,0,E_k\bar{P})$, that corresponds to a "conditional precession" around the z axis. The direction and speed of the rotation depends on the neighbors. If both neighbors are fully polarized at P=+1 (P=-1) the circular frequency of the rotation is $\omega=+2E_k/\hbar$ ($\omega=-2E_k/\hbar$) while in case of oppositely polarized neighbors $\bar{P}$=0 and there is no rotation.

This two basic rotations can be used to implement the MCCNOT operation. It has three inputs: the initial state of the QCA cell and its two neighbors in the 1D cell line. The MCCNOT inverts the polarization of the cell if its left and right neighbors are equally and fully polarized ($\bar{P}$=+2 or -2), and does not have any effect if the polarization of the neighbors are opposite ($\bar{P}$=0).The operation as shown in Fig. 2 is done in three steps: (1) -90° rotation around the *x* axis with $\gamma=\infty$ for time interval $T_1=\pi\hbar/4\gamma$. (2) 0 or 180° rotation around the *z* axis depending on $\bar{P}$ with γ=0 for time $T_2=\pi\hbar/E_k$. (3) -270°(=+90°) rotation around the *x* axis with $\gamma=\infty$ for time $T_3=3\pi\hbar/4\gamma$.

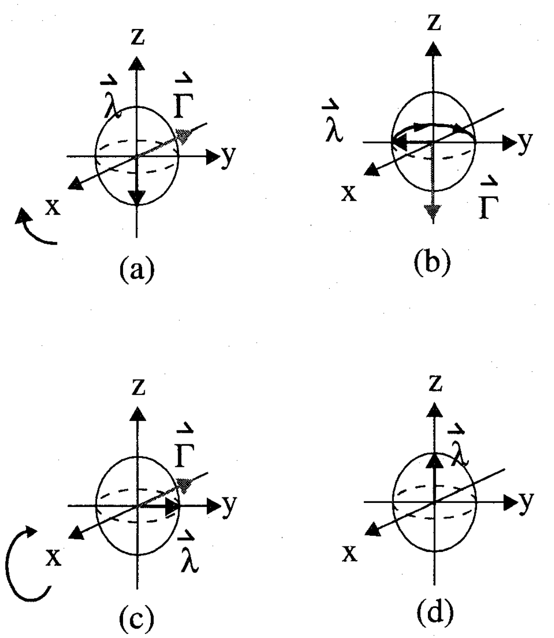

FIGURE 3. The modified controlled controlled NOT (MCCNOT) operation. The two neighbors are supposed to have the same polarization in this example thus the polarization of the cell is inverted. (a) The initial state: $\vec{\lambda}=(0,0,-1)$. It is rotated -90° around the x axis. (b) +180° rotation around the z axis, because the left and right neighbors have the same polarization. If they were different then this rotation would not take place. (c) -270° rotation around the x axis. (d) The final state: $\vec{\lambda}=(0,0,+1)$, and the polarization of the cell is inverted.

The controlled NOT operation can be also realized with QCA cells. It is more complicated than the MCCNOT and explained here only briefly. This operation has two inputs and inverts the first input if the second, so-called control input is P=+1. If the control input is P=-1, the first input remains unchanged. Now the QCA cells are biased by another type of external electrodes. By these electrodes $\overline{P}$ can be much greater than one. Let us consider a two cell group. One cell has $\gamma=0$ while the other goes through the following four steps: (1) -90° rotation around the x axis with $\gamma=\infty$ for time interval $T_1=\pi\hbar/4\gamma$. (2) +90° or -90° rotation around the z axis depending on $\overline{P}$ with $\gamma=0$ for time $T_2=\pi\hbar/2E_k$. (3) +90° unconditional rotation around the z axis with $\gamma=0$ and $\overline{P}=\infty$ for time $T_3=\pi\hbar/2E_k\overline{P}$. (4) -270°(=+90°) rotation around the x axis with $\gamma=\infty$ for time $T_4=3\pi\hbar/4\gamma$.

It is worthwhile to compare the QCA quantum computer realization with the nuclear spin quantum computers [23-26]. The role of the nuclear spin is now played by the coherence vector. The spin of the nucleus is manipulated by a strong constant magnetic field and a weaker alternating one while a QCA implementation uses external electrodes to control the interdot tunneling barrier and determine the time dependence of the Hamiltonian. (However, the same effect could be achieved by electromagnetic pulses, as in the case of any optically driven two-level system.) In case of the spin quantum computer there is a spin-spin coupling while the QCA cells are coupled Coulombically. The classical analogy of a spin-1/2 system is a magnetic dipole. The classical analogy of a QCA cell is an electric quadrupole. The QCA cells are accessible individually.

4. Basic operations with the S-matrix description

In this section the two basic rotations (around the $-x$ and z axes, respectively) and two of the basic operations (NOT and MCCNOT) will be described by the S-matrix description. This description is widely used in the literature [18,21] and fully characterizes the new quantum gates.

The dynamics of the state function is given by the time dependent Schrödinger equation. By integrating the Schrödinger equation and supposing that the Hamiltonian is time independent for 0<t<T, the state at time T can be given as

$$|\Psi(T)\rangle = \exp\left(-i\frac{H}{\hbar}T\right)|\Psi(0)\rangle = S_{\gamma,\,\varphi}|\Psi(0)\rangle$$

where the unitary S-matrix describes the change in state due to the Hamiltonian. It has two variables: γ, the interdot tunneling, and φ, the angle of rotation. The duration can be given with the rotation angle: $T=\varphi/|\vec{\Gamma}|$.

For the $\gamma=\infty$ case and for φ rotation, the S-matrix is given as:

$$S_{\gamma=\infty,\,\varphi} = \begin{bmatrix} \cos\frac{\varphi}{2} & i\sin\frac{\varphi}{2} \\ i\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} \end{bmatrix}$$

(For simplicity, $E_0=0$ was taken.) For the NOT operation $\varphi=\pi$ and

$$S_{NOT} = i\sigma_x$$

Using the above operator as a *logical gate* we find the following state transitions:

$$|1\rangle \Rightarrow i|-1\rangle; \qquad |-1\rangle \Rightarrow i|1\rangle$$

The *quantum gate* operation of the NOT can be demonstrated using a superposition state as input:

$$\frac{1}{5}(3|1\rangle + 4|-1\rangle) \Rightarrow \frac{i}{5}(4|1\rangle + 3|-1\rangle)$$

For the γ=0 case the S-matrix will be given in the three QCA cell product basis with the basis vectors:

$$|-1,-1,-1\rangle, |-1,-1,1\rangle, |-1,1,-1\rangle, \ldots, |1,1,1\rangle$$

In the new basis the S-matrices are 8×8. The following S-matrix is computed from the Hamiltonian of three coupled QCA cells (for shortness, this computation is not written here):

$$S_{\gamma=0,\varphi} = diag(e^{-i\varphi}, 1, e^{i\varphi}, 1, 1, e^{i\varphi}, 1, e^{-i\varphi})$$

The S-matrix of the MCCNOT is given as a series of three rotations:

$$S_{MCCNOT} = \left(S_{\gamma=\infty,\frac{\pi}{2}}\right)\times\left(S_{\gamma=0,\frac{\pi}{2}}\right)\times\left(S_{\gamma=\infty,\frac{7\pi}{2}}\right)$$

The result is the following:

$$S^{abc}_{a'b'c'} = \delta^a_{a'}\delta^c_{c'}\delta^{a\oplus b\oplus c}_{b'}(-1)^{\delta^{abc}_{010}+\delta^{abc}_{101}}$$

where abc and $a'b'c'$ mean the three bit combination determining the column and row of the 8×8 matrix. The δ is one if the value of its two indices are equal, otherwise it is zero. It can be seen that in case of 010 or 101 inputs there is a 180° phase shift, indicated by the -1 term.

5. Conclusions

In this paper a quantum computer architecture was proposed consisting of an 1D array of QCA cells. We have demonstrated how to realize the NOT, the controlled NOT and a three-bit quantum gate, the modified controlled controlled NOT operation. Furthermore, the formulas employed allow us to extend into the dissipation regime.

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