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Thermal effect in quantum-dot cellular automata

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Abstract

We present a theoretical study of thermal effect in quantum-dot cellular automata (QCA). A quantum statistical model has been introduced to obtain the thermal average of polarization of a QCA cell. We have studied the thermal effect on an inverter, a majority gate and planar arrays of different sizes. The theoretical analysis has been approximated for a two-state model where the cells are in any one of the two possible eigenstates of the cell Hamiltonian. Hence, only the ± 1 polarization values are taken into account for the statistical analysis. A numerical computational model has been developed to obtain all possible configurations of the cells in an array. In general, the average polarization of each cell decreases with temperature as well as with the distance from the driver cells. We have found the temperatures for thermal breakdown. The results demonstrate the critical nature of temperature dependence for the operation of QCA.

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Keywords: Quantum-dot cellular automata; Thermal effect; Thermal tolerance; Free energy

1. Introduction

The quantum-dot cellular automata (QCA) is a device paradigm for the nanoscale. It is an architecture for binary computation where electrons are confined in dots in a cell. The charge configuration of electrons in the cell is used to encode and process the binary computation. A basic QCA cell has two extra mobile electrons and is made up of four areas or quantum dots at the corners of a square. The two possible antipodal electron configurations in the dots represent the charge polarizations, $P = +1$ and $P = -1$ of the cell. These two degenerate ground states can be used to encode binary ''1'' and ''0.'' The effect of computation is achieved by the Coulomb interaction between electrons in neighboring

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cells, where the polarization state from one cell is mapped onto the other [1].

During the past decade some of the important aspects of QCA have been demonstrated theoretically. Binary wires, logic gates, adders, inverters [2], simple microprocessors [3] and a serial bit stream analyzer (SBSA) have been designed by suitable arrangements of cells [4]. Recently, theoretical results, such as power gain and dissipation, dissipative and asymmetry dynamics [5,6] adiabatic clocking [7], thermal and defect tolerance [8,9], design and simulation tools, have been reported by various researchers [10]. A hardware description language model also has been introduced for the SBSA [11]. Several key features have been studied experimentally. Experimental demonstrations of wires, logic gates, and power gain in clocked latch and shift register have been reported [12,13]. Cells are made of metal islands coupled by capacitors and tunnel junctions, and operating at sub-Kelvin temperatures. Metal-dot QCA cells are viewed as prototypes for molecular implementation [14].

To date, most of the theoretical investigations have been reported at absolute zero temperature. The theoretical results at non-zero temperatures are very important. The thermal effect may cause the failure of even a geometrically symmetric and perfect device. The study of thermal tolerance will provide guidance for designing a device and operating temperature. Since a physical ground state in an array of cells is mapped onto the logical solution state, the thermal fluctuations may cause excitation and correct logical output may not be obtained. The problem was first perceived by Lent et al. [15]. The group introduced a model that allows the determination of the maximum number of cells in a linear array at a given temperature. It is given by the ratio of the kink energy to its thermal energy. The effect of temperature increases with the linear size of a device. The kink energy of a system remains the same but the entropy changes with the size. As a result, the free energy of the array becomes small, and the system moves toward incorrect logical states [16]. Recently, Ungarelli et al. have studied the thermal behavior of QCA wires and reported that error probabilities depend on the energy splitting between the ground state and first excited state to the thermal energy, $K_{\mathrm{B}}T$ [8]. The excitation energy has to be well above the thermal energy. Hence, it is important to understand the thermodynamic effect and thermal operation limit of a QCA device.

In this article we present a quantum statistical model for cell–cell interaction in QCA and thereby calculate the canonical thermal average of polarization for a cell in an array. We report thermal effect on an inverter, a majority gate, and planar arrays of different sizes. The theoretical analysis has been approximated for a two-state model where the cells are in either of the two possible eigenstates of the (isolated) cell Hamiltonian. In Section 2, we include the theoretical methodology and formalism. Results and discussions are presented in Section 3. Finally, in Section 4, summary and concluding remarks will be included.

2. Theory

Consider a planar QCA array of N cells, each cell containing 5 quantum dots and 2 excess electrons of opposite spins. A planar array of cells is shown in Fig. 1.

The total Hamiltonian for the array is given by

$$\hat{H} = \sum_{m} \hat{H}_m + \sum_{m<p} \hat{V}_{\mathrm{int}}^{m,p}. \tag{1}$$

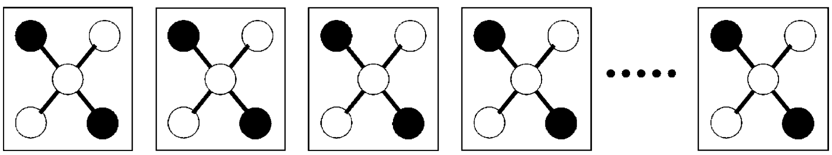

Fig. 1. A QCA array with five dots in each cell.