Finite temperature path-integral modeling of quantum dot cellular automata

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Quantum dot cellular automata (QCA) is a paradigm for nanoscale circuitry [1] that could revolutionize binary computation. It consists of carefully designed structures of quantum dots (QD), where tunneling of single charge carriers is exploited for transmission of information without electric current. However, the development of QCA faces challenges in fabrication techniques and robustness to, e.g., temperature.

Typical building blocks of QCA are rectangular four-site, or four QD, cells with two excess electrons, each. Strong Coulombic correlation forces the electrons to opposite sites [1], see Figure 1. This gives rise to bistable ground state, whose polarization distinguishes the "1" bit from the "0" bit. In suitable composition, the polarization state couples with the neighbouring cells, but this is very susceptible to temperature and other distracting factors, such as fabricational defects. Thus, proper means of modeling QCA are called for.
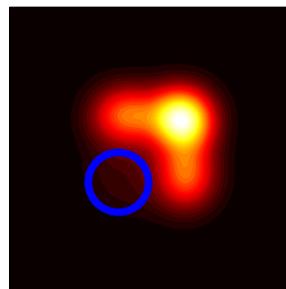

Figure 1: Correlation density of one electron according to the other (blue circle) in a QCA cell with QD size $L = 40$nm, site separation $a = 30$nm and $T = 0.85$K. [3].

Modeling of strongly correlated bistable quantum dot system in finite temperature is hardly accessible by most of the tools in electronic structure computation and quantum chemistry. However, with path-integral Monte Carlo (PIMC) [2] we can access the finite temperature statistics of a QCA cell without any tradeoffs.

With accurate quantitative data from single cell we demonstrate the common dependencies of QCA fidelity on geometry and temperature [3]. Also, beyond the pragmatic QCA design and semi-classical models, we study the regime of significant quantum dot overlap. We find that quantum delocalization has diminutive effect on fidelity, which only wears off in high temperatures, due to quantum decoherence.

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[3] Juha Tiihonen, Andreas Schramm, Ilkka Kylänpää, and Tapio T Rantala. Exact modeling of finite temperature and quantum delocalization effects on reliability of quantum-dot cellular automata. *J. Phys. D: Appl. Phys.*, 49(6):065103, Jan 2016.