Models of Decoherence and Dissipation in QCA Systems

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Quantum-dot cellular automata (QCA) is a novel computing paradigm in which classical bits are encoded using the charge state of a nanostructure known as a QCA cell. A QCA cell is comprised of several quantum dots which localize mobile charge. The intracellular, inter-dot quantum-mechanical tunneling of charge enables device switching. An isolated cell has two degenerate charge configurations which can encode a bit. A network of cells interacts via electric field coupling to lift this degeneracy, enabling general-purpose computing. [1]

The absence of charge transfer between devices makes QCA a low power dissipation computing paradigm. QCA cells and logic devices have been demonstrated in metal-dot implementations at cryogenic temperatures. [2] More recently, a room-temperature QCA cell was implemented using dangling bonds on a H-terminated Si surface. [3] Molecular QCA offer room-temperature operation and synthetic regularity, as well as ultra-high device densities. [4], [5]

We compare models of decoherence and dissipation in QCA systems. A simplified exact model is developed as a fiducial model against which several different approaches to including dissipation and decoherence will be compared.

The exact model includes both the system, a QCA cell, and the environment, modeled as a random arrangment of neighboring cells. The system and environment are treated as a single composite closed system using density matrix formalism in the quantum Liouville equation.

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}_{\mathrm{C}}(t) = \left[\hat{H}_{\mathrm{C}}, \hat{\rho}_{\mathrm{C}}(t)\right] \tag{1}$$

$\hat{H}_{\mathrm{C}}$ is the Hamiltonian for the composite system, and $\hat{\rho}_{\mathrm{C}}(t)$ is the corresponding composite system density matrix. This model provides complete knowledge of the system of interest and the environment but comes with a high computational cost. Figures 1 and 2 show such a simulation.

We consider several models for the Lindblad superoperator $\mathcal{L}(\hat{\rho}_{\mathrm{S}})$. A system of QCA cells is then simulated using the Lindblad form of the quantum master equation.

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}_{\mathrm{S}}(t) = \left[\hat{H}_{\mathrm{S}}, \hat{\rho}_{\mathrm{S}}(t)\right] + \mathcal{L}(\hat{\rho}_{\mathrm{S}}) \tag{2}$$

Here, $\hat{H}_{\mathrm{S}}$ is the Hamiltonian for the open system of interest; $\hat{\rho}_{\mathrm{S}}$ is the reduced density matrix for the system; and $\mathcal{L}(\hat{\rho}_{\mathrm{S}})$ describes the coupling of the environment to the system. Different choices for $\mathcal{L}(\hat{\rho}_{\mathrm{S}})$ correspond to different models for the system-environment coupling and are compared with the results of the exact model.

Acknowledgment

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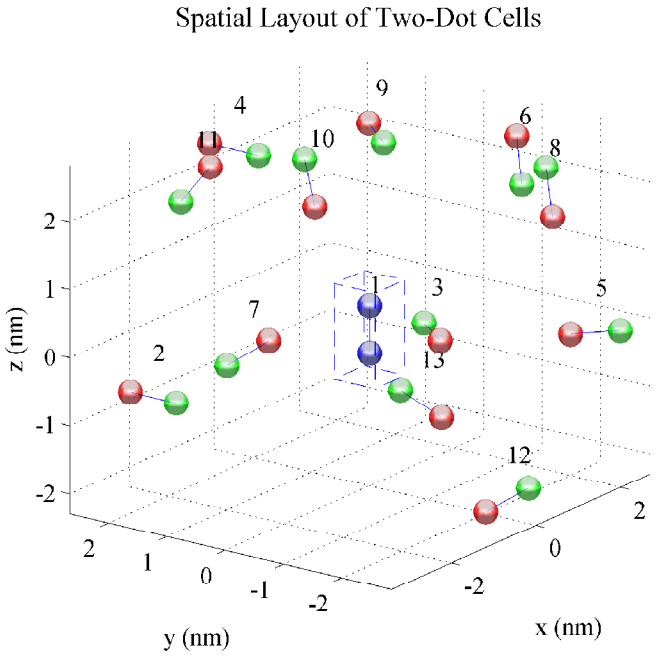

Fig. 1. A target two-dot QCA cell (shown in blue, inside the dashed blue box, numbered "1") is surrounded by a twelve-cell bath. Charge tunneling is not allowed in any of the cells so that no energy can be dissipated from the target cell; however decoherence still occurs.

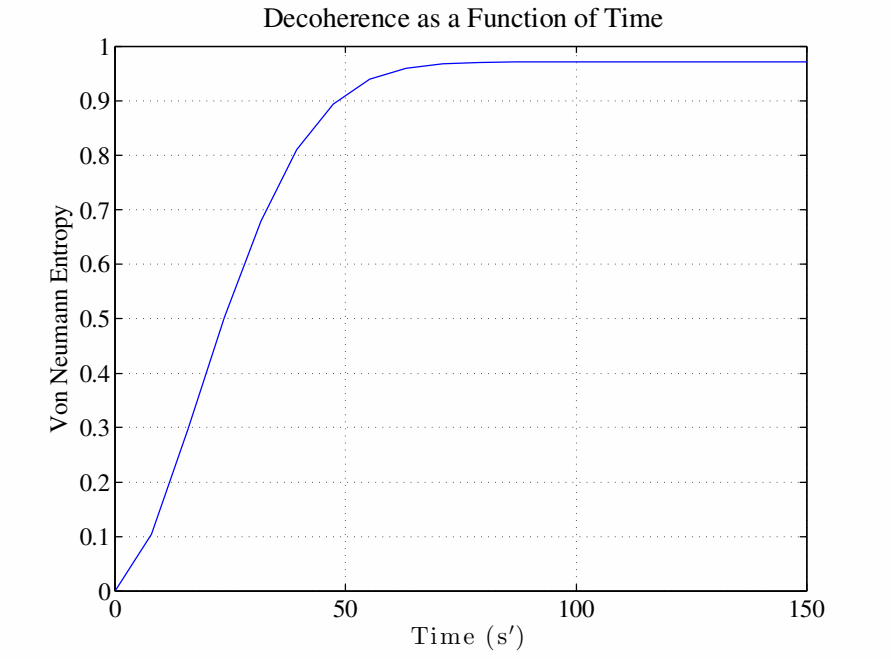

Fig. 2. The array of Figure 1 is simulated using the exact model. Von Neumann entropy is plotted for the target cell, showing the loss of coherence in time. Here, $1\ \mathrm{s}' = 6.582\times10^{-16}$ s. The target cell started in the state given by the coherence vector $\vec{\lambda}_o = (0.6928, -0.6928, 0.2)$. No energy is dissipated from the target cell, so the third component λ_3 of $\vec{\lambda}$ remains constant while $\lambda_1, \lambda_2 \to 0$ so that Von Neuman entropy reaches a non-unity terminal value.