Power Dissipation Bounds and Models for Quantum-dot Cellular Automata Circuits

Saket Srivastava*, Sudeep Sarkar† and Sanjukta Bhanja*
* Electrical Engineering,† Computer Science and Engineering
University of South Florida, Tampa, Florida.
Emails: (ssrivast, bhanja)@eng.usf.edu, sarkar@cse.usf.edu

Abstract— **The goal of this work is to present a worst-case power estimation model for QCA designs. Based on existing power models, we derive upper bound for power dissipation that occurs for non-adiabatic clock switching and represents the worst-case power estimate. This upper bound is easy to compute and does not require simulation of quantum dynamics. Given the criticality of thermal issues and the inherent process variabilities at nano-scale, such worst case estimates, that is easy to compute, will be useful at higher levels of design abstractions, so as to vet different designs or to create power macromodels for different circuit components. There are three power dissipation events for each cell: first when the clock goes up, second when the input switches, and third when the clock goes down. The first and the third events are analogous to "leakage" power in CMOS designs in that there is dissipation even when there is no change in inputs. The second event can be related to "switching" power in CMOS and is dependent on inputs. The proportion between these two types of dissipations is strongly dependent on the clock energy. In addition to the clock, the other determining factors are cell polarization, kink energy, and quantum relaxation time. We demonstrate the model using majority gate and inverter, which are critical circuit components.**

I. Introduction

Quantum-dot cellular automata (QCA) is an emerging technology that offers revolutionary approach to computing at nano-level [1], where computation is performed by device to device Coulombic interaction. Both individual QCA cell (semi-conductor and metallic) and multiple QCA arrangement, such as wire and majority logic, have been fabricated and tested [2]. Significant progress is also being made in using molecules to implement QCAs [3], which will make it possible to operate at room temperature. Since the QCA concept does not involve transfer of electrons, it has a potential for extremely low-power computing, even below the traditional kT in the most optimistic case [4]. However, given that only few electrons are involved in computation, it is susceptible to thermal issues. Hence, it is important to be able to model and predict power dissipated for the worst-case.

Elementary units of a QCA design are the QCA cells that contain two electrons and four possible dot locations at each corner of a QCA cell. There are two ground states of each cell, 0 or 1, and the particular state of a cell is determined by the Coulombic interactions with neighboring cell states. The intended logic is mapped to the ground state of the configuration. While there is no or very little quantum entanglement between cells, there is significant entanglement between the dots within a cell. The extent of the entanglement is determined by the tunneling energy, which is used to depolarize (nullify the cell state) a cell or to latch it into a 0 or 1 state. Current QCA designs rely on a set of 4 clocks, phase shifted with respect to each other, and used to "push" information from inputs to the output by modifying the cell tunneling energy. The complete circuit is divided into zones, each associated with one of the 4 clocks in sequence. The clocks are used to change the state of a cell from a depolarized state to a latching state, to a hold state, and then back to a depolarized state.

While work on issues related to defect and faults in QCA circuits have started [5], power models are few. Timler *et al.* [6] proposed a model to estimate power dissipation during quasi-adiabatic switching event in a QCA cell and demonstrated it for a clocked wire. They showed that when clock changes are nearly adiabatic, i.e. very smooth clocks, then the power loss can be made as low as possible. Our work builds upon this quantum mechanical power model to estimate an easy to compute *upper bound* of power dissipation in QCA circuits as a function of cell polarization, clock energy, kink energy and quantum relaxation time. Unlike Timer *et al.*'s quasi-adiabatic estimate, the computation of this upper bound does not require full quantum-mechanical simulations. Thus, allowing one to quickly form power estimates during the design process. Such upper bound represents the worst-case power dissipation, which happens in the presence of non-adiabatic clocking. Given fabrication variabilities of nano-level components and the importance of thermal issues, it is important to design for the worst-case scenarios. Such estimates, which are easy to compute, will be useful to make design choices at higher levels of design abstractions, as and when they are developed for QCA based circuits.

Each cell in a QCA circuit sees three types of events: (i) clock going from low to high so as to "depolarize" a cell, (ii) input or cells in previous clock zone switching states, and (iii) clock changing from high to low, latching and holding the cell state to the new state. Each of these events are associated with power loss. An interesting point is that the power dissipated in the first and the third transition is due to the clock changing and occurs even if the state of a cell does not change. This is analogous to "leakage" power in CMOS circuits. The power loss due to the second event can be termed as the "switching" power since it is dependent on the cells actually changing state.

The major contributions of this paper are (i) the derivation of the upper-bound or worst-case power dissipation that does require full quantum-mechanical simulation to estimate and

1-4244-0078-3/06/$20.00 (c) 2006 IEEE

(ii) the separation of total power into a "leakage" component and an input dependent "switching" component. We demonstrate our power model by simulating well known basic QCA elements like the inverter and majority gate. We also show how the total power dissipated in a cell varies when the clock energy supplied to it is varied.

II. Upper Bound Power Model

We start with the power formulation in [6] and then derive worst-case estimates by considering the limiting case of non-adiabatic clocking. Two possible, orthogonal, eigenstates of a QCA cell is denoted by $|1\rangle$ and $|0\rangle$. The state or wave function at time t, $|\Psi(t)\rangle$, evolves according to Schrodinger equation, driven by the underlying Hamiltonian $\mathbf{H}$, which is 2 by 2 matrix using the Hartree approximation [1].

$$\mathbf{H} = \begin{bmatrix} -\frac{1}{2}\sum_i E_k P_i f_i & -\gamma \\ -\gamma & \frac{1}{2}\sum_i E_k P_i f_i \end{bmatrix} = \begin{bmatrix} -\frac{1}{2}E_k\bar{P} & -\gamma \\ -\gamma & \frac{1}{2}E_k\bar{P} \end{bmatrix} \tag{1}$$

The expected value of any observable, $\langle\hat{A}(t)\rangle$, can be expressed in terms of the wave function as $\langle\hat{A}\rangle = \langle\Psi(t)|\hat{A}(t)|\Psi(t)\rangle$ or equivalently as $\mathrm{Tr}[\hat{A}(t)|\Psi\rangle(t)\langle\Psi(t)|]$, where Tr denotes the trace operation, $\mathrm{Tr}[\cdots] = \langle 1|\cdots|1\rangle + \langle 0|\cdots|0\rangle$. The term $|\Psi(t)\rangle\langle\Psi(t)|$ is known as the density operator, $\hat{\rho}(t)$. Expected value of any observable of a quantum system can be computed if $\hat{\rho}(t)$ is known.

Energy (and power) can be estimated by computing the expected Hamiltonian using this density matrix. However, for compact mathematical representation of power dissipation the Bloch formulation of the Schrodinger equation, which expresses the evolution of quantum systems in operator spaces, is used. In this formulation, the expectated value of cell energy $\langle\hat{\mathbf{H}}\rangle$ at any time is given by:

$$E = \langle\hat{H}\rangle = \frac{\hbar}{2}\vec{\Gamma}.\vec{\lambda} \tag{2}$$

where $\vec{\Gamma}$ and $\vec{\lambda}$ are the Hamiltonian and coherence (state) vectors respectively. These are arrived at by expressing the density operator as a linear combination of the Pauli's spin operator σ_i: $\rho(\mathbf{t}) = \sum_{i=1}^{3}\lambda_i\sigma_i$, where $\lambda_i = Tr\{\hat{\rho}\hat{\sigma}_i\}$. The two state Schrodinger Hamiltonian can be projected onto the Pauli basis of generators to form a real three-dimensional energy vector $\vec{\Gamma}$, whose components are $\Gamma_i = \frac{Tr\{\hat{H}\hat{\sigma}_i\}}{\hbar}$. The explicit form of the Hamiltonian vector corresponding to Hamiltonian is

$$\vec{\Gamma} = \frac{1}{\hbar}\begin{bmatrix} -2\gamma, 0, E_k\bar{P} \end{bmatrix} \tag{3}$$

where $\bar{P}$ is the sum of neighboring polarizations. The instantaneous power dissipation in a single QCA cell is

$$P = \frac{dE}{dt} = \frac{\hbar}{2}\left[\frac{d\vec{\Gamma}}{dt}.\vec{\lambda}\right] + \frac{\hbar}{2}\left[\vec{\Gamma}.\frac{d\vec{\lambda}}{dt}\right] = P_1 + P_2 \tag{4}$$

The term P_1 includes power from clock introduced into the cell P_{clock} and power gain from input to output $(P_{in} - P_{out})$ [6]. We are concerned with $P_2 = P_{diss}$ which represents the instantaneous dissipated power. We use this expression for this power dissipation equation to arrive at a bound.

We express the energy dissipated by integrating P_{diss} over time.

$$E_{diss} = \frac{\hbar}{2}\int_0^\infty \vec{\Gamma}.\frac{d\vec{\lambda}}{dt}.dt \tag{5}$$

Integrating by parts, we get:

$$E_{diss} = \frac{\hbar}{2}\left[\vec{\Gamma}(\infty).\vec{\lambda}(\infty) - \vec{\Gamma}(0).\vec{\lambda}(0) - \int_0^\infty \vec{\lambda}(t).\frac{d\vec{\Gamma}(t)}{dt}.dt\right] \tag{6}$$

The dissipation is related to the rate of change of Γ, which as we see in Eq. 3, is determined by the clock and neighboring polarizations. The faster the rate of change, the more is the dissipated energy. In the limiting case of abrupt switching, the energy dissipation will be the largest, which will be the upper bound. We capture this abrupt switching case by modeling the $\frac{d\vec{\Gamma}(t)}{dt}$ term using delta function as $\Delta\vec{\Gamma}.\delta(t)$, where $\Delta\vec{\Gamma} = (\vec{\Gamma}_{0^+} - \vec{\Gamma}_{0^-})$ – the difference in magnitude of clock and/or neighboring polarizations before and after the switching event. Therefore the integral term in the above equation reduces to:

$$\begin{aligned} \int_0^\infty \vec{\lambda}(t).\frac{d\vec{\Gamma}(t)}{dt}.dt &= \int_0^\infty \vec{\lambda}(t).\Delta\vec{\Gamma}.\delta(t)dt \\ &= \left[\vec{\Gamma}(\infty) - \vec{\Gamma}(0)\right].\vec{\lambda}(0) \end{aligned} \tag{7}$$

Using Eqs. 5 and 7 we can now represent the dissipation energy explicitly in terms of coherence vector $\vec{\lambda}(t)$ and Hamiltonian vector $\vec{\Gamma}(t)$ as

$$E_{diss} = \frac{\hbar}{2}\left\{\vec{\Gamma}(\infty).[\vec{\lambda}(\infty) - \vec{\lambda}(0)]\right\} \tag{8}$$

The steady state density matrix at thermal equilibrium is

$$\hat{\rho}_{ss} = \frac{e^{-H/k_BT}}{Tr\{e^{-H/k_BT}\}} \tag{9}$$

The associated steady state coherence vector is

$$\vec{\lambda}_{ss} = -p = -\frac{\vec{\Gamma}}{|\vec{\Gamma}|}\tanh(\Delta) \tag{10}$$

where the temperature ratio (Δ) is defined as

$$\Delta = -\frac{\hbar|\vec{\Gamma}|}{2k_BT} \tag{11}$$

Using these Eqns. 9, 10 and 11 we obtain the values of $\vec{\lambda}(\infty)$ and $\vec{\lambda}(0)$

$$\begin{aligned} \vec{\lambda}(\infty) &= -\frac{\vec{\Gamma}_{new}}{|\vec{\Gamma}_{new}|}\tanh(\Delta_{new}) \\ \vec{\lambda}(0) &= -\frac{\vec{\Gamma}_{old}}{|\vec{\Gamma}_{old}|}\tanh(\Delta_{old}) \end{aligned} \tag{12}$$

where $\vec{\Gamma}_{new}$ and $\vec{\Gamma}_{old}$ correspond to the values $\vec{\Gamma}_{0^+}$ and $\vec{\Gamma}_{0^-}$ respectively during the abrupt (non-adiabatic) switching. Now rearranging Eq. 10 we get

$$\tanh(\Delta) = \frac{p\,\hbar}{E_k\bar{P}}|\vec{\Gamma}| \tag{13}$$

Using these expression we can now express the upper bound of cell energy dissipated during each switching event of the inputs as a function of before and after polarizations of the

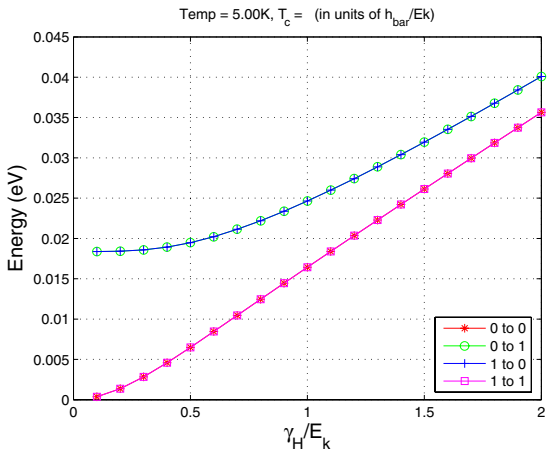

Fig. 1. Dependence the total energy dissipated in a cell with clock energy for different clock transitions. (a) 0→0 (b) 0→1 (c) 1→0 and (d) 1→1. Note that the plots for cases (a) and (d) overlap completely and so does the plots for cases (b) and (c).

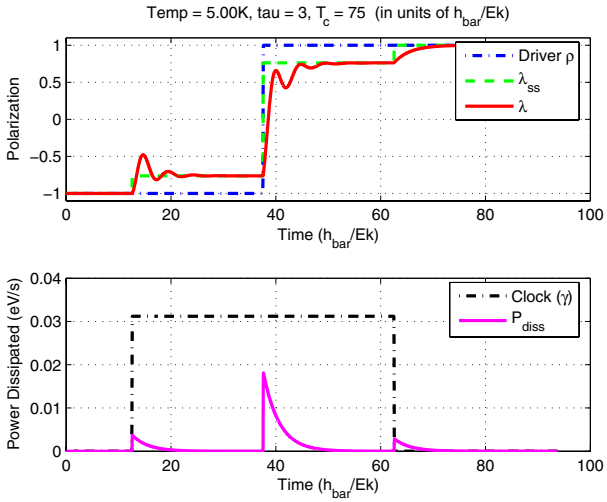

Fig. 2. Polarization change (top plot) and power loss (bottom plot) in a single cell when its polarization changes from -1 to 1 (or 0 to 1 logic) during non-adiabatic clocking scheme

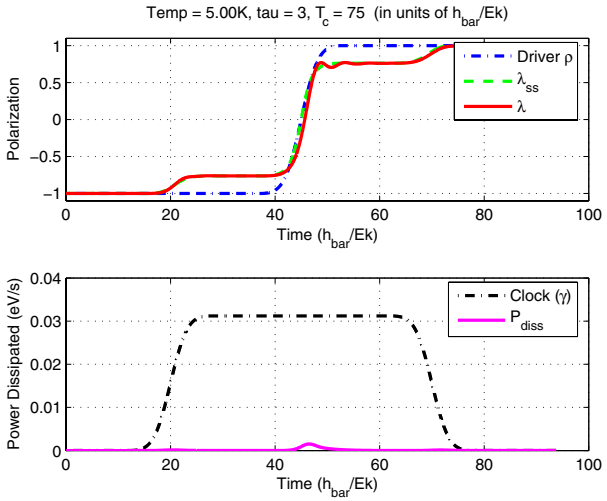

Fig. 3. Polarization change (top plot) and power loss (bottom plot) in a single cell when its polarization changes from -1 to 1 (or 0 to 1 logic) during a quasi-adiabatic clocking scheme.

cells. Given a circuit, these cell polarization changes can be easily computed.

$$E_{diss} \leq \left[\frac{2\gamma_{new}}{E_k}\left(\frac{p_o}{\bar{P}_{old}}\gamma_{old} - \frac{p_n}{\bar{P}_{new}}\gamma_{new}\right) + \frac{E_k\bar{P}_{new}}{2}(p_o - p_n)\right] \tag{14}$$

Fig. 1 shows how the total dissipated energy changes when the clock energy supplied to the cell is increased from $0.05E_k$ to $2E_k$ for different state transitions (a) 0→0 (b) 0→1 (c) 1→0 and (d) 1→1. Here E_k is the maximum value of kink energy between any two cells in the circuit. Note that energy is dissipated even if the state of a cell does not change, i.e for cases (a) and (d). This is because the high clock state only *partially* depolarizes a cell and there is change in this partial polarization with input change. As the high clock energy is increased, the cell gets depolarized to a greater extent and the contribution to overall dissipation due to switching states is less. However, as we see in Fig. 1, the total dissipated energy also increases; this is due to the contribution of dissipative event associated with clock transitions, i.e. "leakage power." So, we cannot increase clock energy indefinitely.

If τ is the energy relaxation time, using Eq. 2 we can represent the power dissipated in a QCA cell by:

$$P = \frac{\hbar}{2\tau}(\vec{\Gamma}(\vec{\lambda} - \vec{\lambda_{ss}})) \tag{15}$$

Similar to Eq. 14 we can now find the upper bound of power dissipated at each cell in a QCA logic circuit as

$$P_{diss} \leq \frac{1}{\tau}\left[\frac{2\gamma_{new}}{E_k}\left(\frac{p_n}{\bar{P}_{new}}\gamma_{new} - \frac{p_o}{\bar{P}_{old}}\gamma_{old}\right) + \frac{E_k\bar{P}_{new}}{2}(p_n - p_o)\right] \tag{16}$$

III. Results

We first validate our power bound expressions using quantum simulation of single cells. Then we show how we can use these bounds to compute worst case power dissipation for collections of cells. Fig. 2 shows the switching behavior and power dissipation during a non adiabatic change in polarization of a cell being driven by a single input. As we can see from the graph, the steady state polarization λ_{ss} of the cell follows the driver polarization. In the ideal case of adiabatic switching, the polarization of the cell (λ) should trace the same curve as λ_{ss}. But as we see, that this is not the case, since due to this abrupt switching, the polarization of cell takes some time to settle down to a steady state value. As we can see from the graphs, the total power dissipated by the cell occurs not only when its polarization changes, but a significant amount of power loss also occurs when the clock energy barriers are raised and lowered. We verified the total energy computed using these types of quantum simulation with theoretical bounds and found them to be in perfect agreement.

As a comparison, Fig. 3 shows the same switching event as in Fig. 2 but with a quasi-adiabatic clocking scheme with smoothed clock transitions. As we can see from the figure, for quasi-adiabatic switching the power loss due to clock

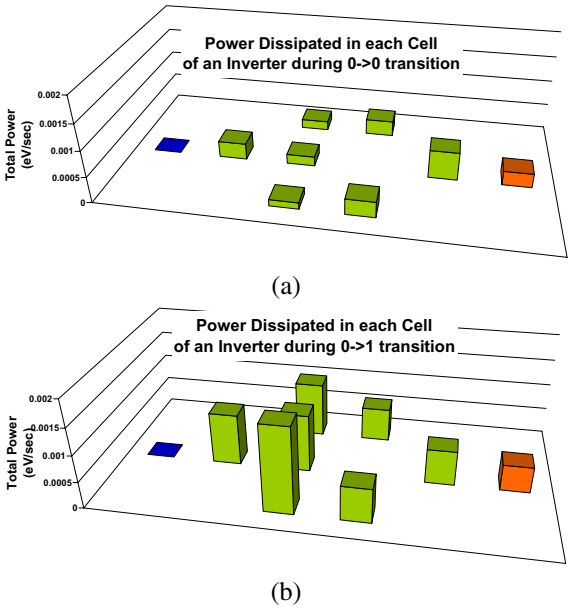

Fig. 4. Total power dissipated in each cell of a QCA Inverter for (a) 0→0 input transition (b) 0→1 input transition.

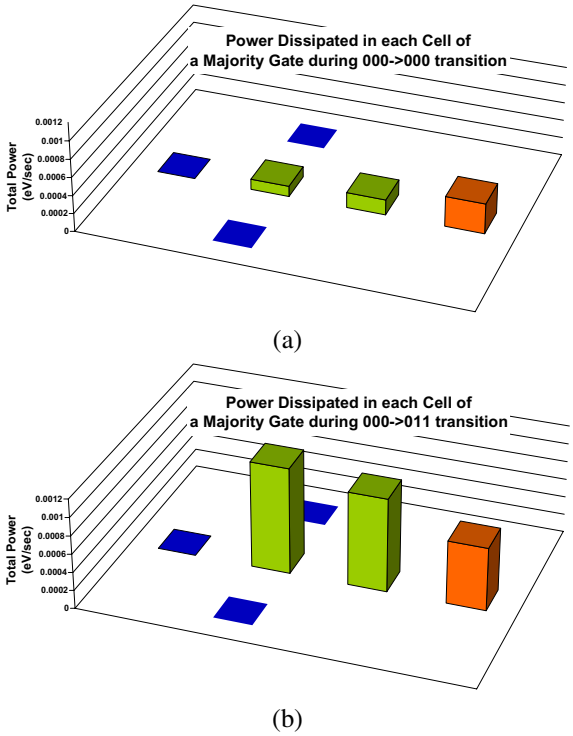

Fig. 5. Power dissipated in each cell of a QCA majority gate for (a) no input transition 000→000 and (b) input transition 000→011.

switching is almost zero and power loss due to change in polarization of the cell is reduced significantly. For ideal adiabatic switching, which is not practical though, there should be no power loss.

Next, we consider some arrangements of QCA cells implementing crucial QCA circuit elements. Fig. 4 shows the power loss at each cell of an inverter when the polarization of the input cell is (a) kept constant 0→0 and (b) changed 0→1. For this work, we have taken the value of high clock to be $0.7E_k$. Where E_k is the maximum value of kink energy between any two cells in the circuit. As can be predicted when there is no change in input polarization (0→0 transition), the total power dissipated each cell will be only due to the raising and lowering of clock barriers.

Fig. 5 show the power dissipated in the cells of a majority gate whenever its inputs are (a) not switched 000→000 and (b) switched 000→011. We have observed some interesting results while studying various input vector transitions in a majority gate. While we have seen that in case no switching, i.e. 000→000, there is no change in polarization of the cells and hence the total power dissipated is equal to the power dissipated in raising and lowering the clock energy barriers. In case of a 000→011 transition shown in Fig. 5(b), the total power dissipation in each cell will be significantly higher as there is significant amount of power dissipation when the polarization of cell changes. As we can see clearly from the power dissipation graphs of inverter and majority gate, the total power dissipation in an inverter is larger as compared to that of a majority gate. Also the value maximum power dissipated in single cell in an inverter seems to be larger than that of a majority gate. For thermal stability of designs, it would be important to consider the maximum power dissipated at any cell in a design. Two designs might have the same total power, but the maximum power at any cell might be higher in one design.

IV. Conclusion

We developed a worst-case power dissipation model for QCA circuits based on the non-adiabatic case associated with abrupt clock switching. We derived theoretical upper bounds on dissipated power and then established correspondence with the concepts of "leakage" and "switching" power in CMOS circuits. Such separation is quite important for circuit designs since switching power is dependent on the circuit input patterns, while leakage power is independent of inputs. The main contribution of this work is that we can compute power dissipated at each individual cell in a circuit for any input vector transition. This enables us to locate cells in a circuit that are critical in terms of power dissipation and also the input vector transitions that result in large power dissipations. One important observation of this work is the extent to which clock energy has an impact on the power dissipated in QCA circuits.

References

[1] C. Lent and P. Tougaw, "A device architecture for computing with quantum dots," in *Proceeding of the IEEE*, vol. 85-4, pp. 541–557, April 1997.

[2] A. Orlov, R. Kummamuru, R. Ramasubramaniam, C. Lent, G. Bernstein, and G. Snider, "Clocked quantum-dot cellular automata shift register," *Surface Science*, vol. 532, pp. 1193–1198, 2003.

[3] C. Lent, B. Isaksen, and M. Lieberman, "Molecular quantum-dot cellular automata," *Journal of American Chemical Society*, vol. 125, pp. 1056–1063, 2003.

[4] J. Timler and C. Lent, "Maxwell's demon and quantum-dot cellular automata," *Journal of Applied Physics*, vol. 94, pp. 1050–1060, July 2003.

[5] M. Tahoori, J. Huang, and F. Momemjadeh, M. Lombardi, "Testing of quantum cellular automata," *IEEE Transactions on Nanotechnology*, vol. 3, no. 4, pp. 432–442, 2004.

[6] J. Timler and C. Lent, "Power gain and dissipation in quantum-dot cellular automata," *Journal of Applied Physics*, vol. 91, pp. 823–831, January 2002.