"Single-Electron Parametron": Reversible Computation in a Discrete-State System

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The energy dissipation in a proposed digital device in which discrete degrees of freedom are used to represent digital information (a "single-electron parametron") was analyzed. If the switching speed is not too high, the device may operate reversibly (adiabatically), and the energy dissipation $\mathcal{E}$ per bit may be much less than the thermal energy scale k_BT (where k_B is Boltzmann's constant and T is temperature). The energy-time product $\mathcal{E}\tau$ is, however, much greater than Planck's constant $\hbar$, at least in the standard "orthodox" model of single-electron tunneling that was used in these calculations.

Computation always leads to energy dissipation because of the unavoidable coupling between the degrees of freedom that represent information and the environment. In most practical electronic devices (such as semiconductor transistor circuits), energy is dissipated at some rate even when no information processing occurs. However, some proposed digital devices, such as various single-flux–quantum (*1*, *2*) and single-electron (*3*, *4*) logics, do not involve static power consumption because they represent conservative systems in which digital information is coded by the choice of a local minimum of potential energy (*5*). In this case, the energy dissipation is proportional to the number of logic operations. If such a conservative system is switched irreversibly (*2*), the energy loss $\mathcal{E}$ per logic operation is of the order of the energy barrier W separating the states. The barrier should be sufficiently high to make the probability $p \sim \exp(-W/k_BT)$ of thermally induced errors low enough, so that at the physically irreversible computation $\mathcal{E}_{min} \sim k_BT \ln(1/p) \gg k_BT$.

Some conservative systems, such as the parametric quantron (PQ) (*1*, *6*), are flexible enough to allow independent adjustment of the potential tilt and barrier height. This flexibility allows physically reversible (adiabatic) switching of the system with $\mathcal{E} \ll k_BT$ if the information content of the system remains intact (*7*, *8*). If, however, information is lost during the operation (informationally irreversible computation), the energy loss is at least $\mathcal{E}_{min} = k_BT \ln 2$ per each lost bit. Thus, $\mathcal{E}$ may be made much less than k_BT only for completely (physically and informationally) reversible computation. In this case, $\mathcal{E}$ scales as τ^{-1}, where τ is the switching time, so that the product $\mathcal{E}\tau$ is fixed (*7*).

The quantity $\mathcal{E}\tau$ has the dimensionality of $\hbar$, so the natural question is whether quantum mechanics imposes any fundamental lower bound on this product. A quantitative analysis of the reversible PQ system has shown (*9*) that $\mathcal{E}\tau$ may be much less then $\hbar$. However, that analysis assumed that the potential energy is a function of a continuous degree of freedom (in that particular case, the Josephson phase ϕ). To our knowledge, a similar analysis has not been carried out for any system that represents information with discrete states.

Recently we suggested (*10*) a system (single-electron parametron), based on correlated single-electron tunneling (*3*), that may be used for reversible computation with a discrete degree of freedom: the electric charge Q. In the present work, our goal was to find the minimum energy dissipation $\mathcal{E}$ for this system and to relate it to the switching time τ and to the error probability p. In particular, we have shown that, within the "orthodox" theory (*11*), $\mathcal{E}\tau$ is always considerably larger than $\hbar$.

The possible structure of a unit cell of the system is shown in Fig. 1A. It consists of at least three small conducting islands (with capacitances $C \ll e^2/k_BT$, where e is the electron charge), with the middle island slightly shifted in the y direction. Tunnel barriers with small conductances ($G \ll e^2/\hbar$) allow direct transfer of electrons only between the neighboring islands. The system is biased by a periodic ("clock") electric field $\mathbf{E}(t)$ perpendicular to the x axis. Let us consider the conceptually simplest case, in which the cell is charged as a whole by a single extra electron. [In practice, operation with electron-hole pairs may be beneficial (*10*, *12*), but for this discussion both versions are identical.]

When the vertical component $E_y(t)$ of the field is lower than a certain threshold value E_t, the extra electron is kept inside the middle island. The energy diagram for this OFF state is shown in the upper panel of Fig. 1B. As E_y is increased, the tunneling of the electron from the middle island into one of the edge islands becomes energy-advantageous at $E_y > E_t$. If the system is completely x-symmetric, this results in spontaneous symmetry-breaking, so that the direction of the resulting electric dipole moment P_x of the system is random: $P_x = Qd_{eff}$, $d_{eff} \approx d$, $Q = \pm e$. However, if the symmetry is broken by a weak additional external field E_x (induced, for example, by the dipole moment of a similar neighboring cell), the direction of the electron tunneling (and hence the sign of P_x) is predetermined by this field. The middle panel of Fig. 1B shows this OFF → ON switching stage.

When E_y is well above E_t, the electron is trapped inside one of the edge islands, even if the signal field E_x now favors its transfer in the opposite edge direction (ON state; lower panel of Fig. 1B). In this state, electron transfer may only be achieved through a higher order "cotunneling" process; the probability of this process may be made negligibly small either by decreasing the tunnel conductance or by inserting a few additional islands into the cell (*11*). If this parasitic process is negligible, the cell has a fixed dipole moment and may serve as a robust source of signal field E_x for similar neighboring cells. After this source has been used, the system is reset into the OFF

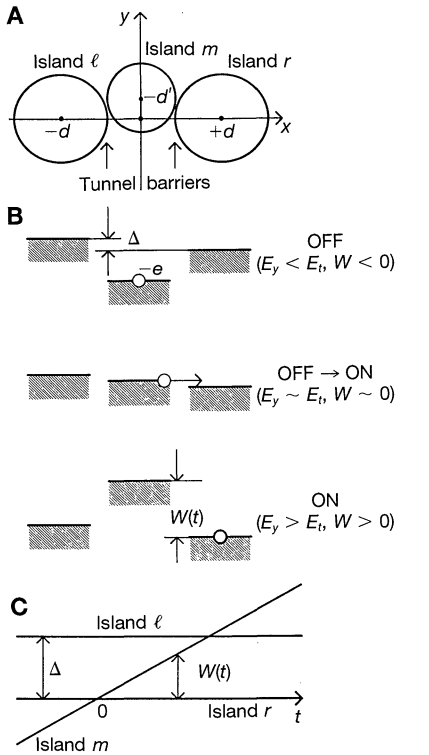

Fig. 1. The single-electron parametron: (**A**) three-island version of the system; (**B**) its energy diagram for three values of the clock field E_y; and (**C**) energy of the extra electron in various islands as a function of time, close to the decision-making moment $t \approx 0$.

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state during the corresponding part of the clock cycle, when $E(t)$ again drops below E_t.

The operation of the cell is quite similar to that of the PQ (*1*), except that now the information is represented by a discrete variable, $Q = \pm e$. In particular, the parametron may be used for reversible transfer and processing of information (*10*, *12*). A possible structure of a shift register is shown in Fig. 2. In each neighboring cell, the extra charge sign alternates, while the direction of the middle-island shift within plane yz is changed by $\Theta = \pi - 2\pi/M$, where $M > 2$ is the number of cells per bit (in Fig. 2, $M = 3$). The clock field $\mathbf{E}(t)$ has a fixed magnitude $E > E_t$ but rotates within the plane yz to provide periodic switching ON and OFF of the cells, with the phase shift $2\pi/M$ between the neighboring cells. At an appropriate choice of E and of distance between the cells (*12*), the orientation of the dipole moment of the cells in the ON state determines the direction of the field E_x and hence the direction of electron tunneling in the neighboring cell that is being switched OFF → ON. As a result, the information is being rewritten from cell to cell and is thus transferred over M cells during each clock period. Reversible logic operations may be implemented in a similar way, for example, by the use of majority gates with additional output cells (*9*).

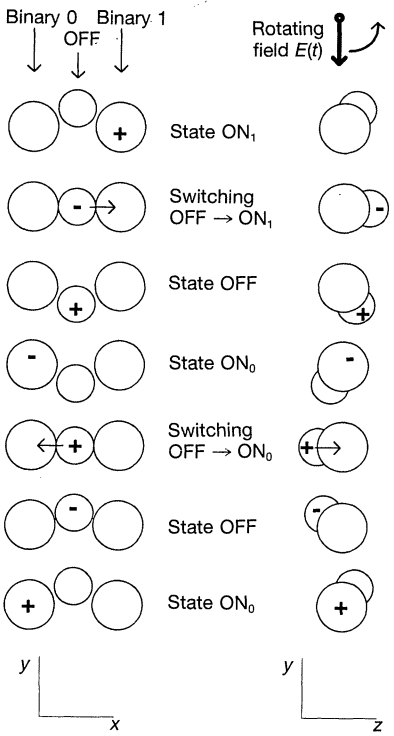

Fig. 2. Top (left) and side (right) views of a shift register with an array of the parametron cells. The clock field $E(t)$ rotates in the yz plane. Digital bits are coded by the positions of the extra charges in the ON state of the cells and are propagated from the top to the bottom, over $M = 3$ cells during one clock period.

Within the orthodox theory (*11*), all properties of the system may be found by solving the system of master equations for the probabilities $p_i(t)$ to find the extra electron in the middle ($i = m$), left ($i = \ell$), and right ($i = r$) islands:

$$\frac{d}{dt}\,p_i = \sum_{j=m,\ell,r} (p_j\Gamma_{ji} - p_i\Gamma_{ij}) \qquad (1)$$

$$\sum_i p_i(t) = 1,\ p_m(0) = 1$$

where in our case the tunneling rate matrix $\mathbf{\Gamma}$ has only four nonvanishing components,

$$\Gamma^{\pm}_{mr} = \frac{\pm GW}{e^2[1 - \exp(\mp W/k_BT)]} \qquad (2)$$

$$\Gamma^{\pm}_{m\ell} = \frac{\pm G(W - \Delta)}{e^2\{1 - \exp[\mp(W - \Delta)/k_BT]\}}$$

Here $\Gamma^{+}_{ij} \equiv \Gamma_{ij}$, $\Gamma^{-}_{ij} \equiv \Gamma_{ji}$, and $W(t) \approx E_y(t)d'$ is the energy difference between the charge configurations with the extra electron in the middle and right islands; $\Delta = 2d_{\text{eff}}E_x$ is the energy difference between the left and right ON states. We assume that, near the decision-making point of the ON → OFF switching ($t \approx 0$ in Fig. 1C), the difference is a linear function of time: $W = \alpha t$. At the decision-making moment, the energy difference Δ should be large enough for the system to operate with a low error probability ($p \ll 1$). Without loss of generality, we may assume $\Delta > 0$; then p can be found from the solution of the master equation as $p_\ell(\infty)$, and the average energy $\mathscr{E}(t)$ dissipated by moment t can be calculated as

$$\mathscr{E}(t) = \int_{-\infty}^{t} \left\{ W(t)\frac{dp_r}{dt} + [W(t) - \Delta]\frac{dp_\ell}{dt} \right\} dt \qquad (3)$$

We will be most interested in the net dissipation $\mathscr{E} \equiv \mathscr{E}(\infty)$.

The solution of Eqs. 1 through 3 yields the following results. With an accuracy sufficient for our final result, the total error probability p may be calculated as a maximum of probabilities of the thermal and dynamic errors. The thermal error may occur as a result of thermally activated tunneling to the wrong state (in this case, ℓ), and its probability p_{therm} can always be expressed as $\exp(-\Delta/k_BT)$. (For this reason, we will restrict our discussion to the limit $\Delta \gg k_BT$.) The dynamic error occurs when the switching speed α is too high, and the system remains in the initial (symmetric) state up to the moment when tunneling to the upper energy level becomes possible. If $\delta \equiv \alpha e^2/G\Delta k_BT \gg 1$, the dynamic error dominates and its probability is given by the expression

$$p_{\text{dyn}} = K\gamma \exp\left(-\frac{1}{2\gamma}\right)$$

$$K = \frac{1}{2\gamma} - \frac{\sqrt{\pi}}{4\gamma^{3/2}} \exp\left(\frac{1}{4\gamma}\right)\left[1 - \text{Erf}\left(\frac{1}{2\sqrt{\gamma}}\right)\right]$$

$$= 1 + \sum_{n=1}^{\infty} \frac{(2n+1)!}{n!}(-\gamma)^n \qquad (4)$$

where $\gamma \equiv \alpha e^2/G\Delta^2$. If $p_{\text{dyn}} \ll 1$ is to be maintained, γ should be $\ll 1$, so that Eq. 4 can be used with $K = 1$.

Energy dissipation depends on another dimensionless parameter,

$$\beta \equiv \alpha e^2/G(k_BT)^2$$

$$= (\Delta/k_BT)^2\gamma = (\Delta/k_BT)\delta \qquad (5)$$

Like γ and δ, the β parameter is also proportional to the switching speed α but β is much larger than both γ and δ (because $\Delta \gg k_BT$) and may be comparable to unity. In the low-speed limit $\beta \ll 1$, the switching process is adiabatic. It consists of numerous tunneling events (back and forth between m and r) taking place within the energy interval $\sim k_BT$ around the point $W(t) = 0$. In this case, $\mathscr{E} = \kappa\beta k_BT$, where

$$\kappa = \int_{-\infty}^{\infty} \frac{e^x(e^x - 1)}{x(1 + e^x)^3}\,dx \simeq 0.426 \qquad (6)$$

so that for this (almost reversible) process $\mathscr{E} \ll k_BT$. Note that $\mathscr{E} = \kappa\beta k_BT = \kappa\alpha e^2/Gk_BT$ decreases when temperature increases.

Our model allows us not only to calculate the net dissipation $\mathscr{E}$ but also to follow the time dynamics of energy transfer between the system and the environment ("heat bath") during the switching process. During the first half of the adiabatic switching process [when $W(t) \le 0$], the energy $\mathscr{E}_1 \equiv -\mathscr{E}(0) = k_BT \ln 2$ is borrowed from the heat bath (which, hence, is cooled), while virtually the same amount $\mathscr{E}_2 \equiv \mathscr{E} - \mathscr{E}(0)$ is returned back to the heat bath during the second half of the process [$W(t) \ge 0$]. This exchange is directly related as $\mathscr{E}(t) = T\Delta S(t)$ to the temporal increase and consequent decrease of the entropy S corresponding to the degree of freedom used to code information (in this particular case, the diploe moment P_x). At the moment when $W = 0$, the system may be in either of two states ($p_m = p_r = \frac{1}{2}$), hence $\Delta S = k_B \ln 2$ has been acquired in comparison with the definite initial state ($p_m = 1$, $p_r = 0$). By the end of the switching ($W \gg k_BT$), S is restored to the initial value because the state is definite again ($p_m = 0$, $p_r = 1$). Finite switching speed decreases $\mathscr{E}_1$ and increases $\mathscr{E}_2$ (see the short-dashed lines in Fig. 3), leading to pos-

itive total dissipation $\mathscr{E} = \mathscr{E}_2 - \mathscr{E}_1$ (*13*).

In the limit $\beta \gg 1$, the speed of energy change is so high that switching may take place only at $W > 0$, but within a much larger interval of energies: $\Delta W \sim \beta^{1/2} k_B T$. The average energy dissipation for this (irreversible) process is of the same order, that is, much greater than $k_B T$ and independent of T: $\mathscr{E} = (\pi\beta/2)^{1/2} k_B T = (\pi e^2 \alpha / 2G)^{1/2}$. The results of numerical calculation of $\mathscr{E}$ for intermediate values of β are represented by the solid line in Fig. 3. Taking into account that at $p \ll 1$ the parameter $\tau = \Delta/\alpha$ may be considered as the duration of the switching process (Fig. 1C), we find that all our asymptotic results can be summarized as follows:

$$\mathscr{E}\tau = \frac{\hbar}{GR_Q} \times \begin{cases} 0.67 \ln(1/p) \text{ for } \delta,\beta \ll 1 \\ 1.97\, \beta^{-1/2} \ln(1/p) \text{ for } \delta \ll 1 \ll \beta \\ 2.78 \left[\ln \dfrac{1}{2p \ln(1/p)} \right]^{1/2} \text{ for } 1 \ll \delta,\beta \end{cases} \quad (7)$$

where $R_Q = \pi\hbar/2e^2 \approx 6.45$ kilohms is the quantum unit of resistance. Because the orthodox theory is valid only at $GR_Q \ll 1$, within this theory $\mathscr{E}\tau \gg \hbar$ for any switching speed.

Our results demonstrate that reversible computation for which the energy dissipation $\mathscr{E}$ per bit is much less than $k_B T$ may be implemented in a physical system with discrete states. However, the quantum bound for the product $\mathscr{E}\tau$ obtained within our concrete model is much greater than that obtained earlier for a system with a continuous degree of freedom (*9*). It is possible that the $\hbar$ limit for $\mathscr{E}\tau$ may be overcome in the case of islands with discrete spectra of electron energies (*14*).

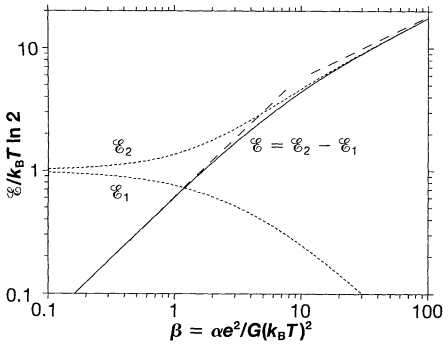

Fig. 3. Components of the energy exchange between the parametron and the heat bath as functions of the process speed $\alpha = dW/dt$. Short-dashed lines represent the average energy flow $\mathscr{E}_1$ from the heat bath to the parametron during the first half of the process ($W \leq 0$) and the average flow $\mathscr{E}_2$ from the device back into the heat bath during its second half ($W \geq 0$), respectively. The solid line denotes the net energy dissipation $\mathscr{E} = \mathscr{E}_2 - \mathscr{E}_1$. The long-dashed line segments show the low-speed (adiabatic) and high-speed (diabatic) asymptotes of the function $\mathscr{E}(\alpha)$ (see equations in the text).

REFERENCES AND NOTES

1. K. K. Likharev, *IEEE Trans. Magn.* **13**, 242 (1976).
2. _____ and V. K. Semenov, *IEEE Trans. Appl. Supercond.* **1**, 3 (1991).
3. D. V. Averin and K. K. Likharev, in *Single Charge Tunneling*, H. Grabert and M. H. Devoret, Eds. (Plenum, New York, 1992), pp. 311–332.
4. A. N. Korotkov, *Appl. Phys. Lett.* **67**, 2412 (1995).
5. We consider only the case in which the state of the system can be described as a classical variable, in contrast to so-called "quantum computing devices" [for example, see I. L. Chuang, R. Laflamme, P. W. Shor, W. H. Zurek, *Science* **270**, 1633 (1995) and references therein]. These "classical" systems (whose dynamics may nevertheless require quantum-mechanical descriptions) may provide reliable computation even at substantial coupling to the environment.
6. This system was reinvented later as a "flux quantum parametron" [see K. F. Loe and E. Goto, *IEEE Trans. Magn.* **21**, 884 (1985)].
7. R. Landauer, *IBM J. Res. Dev.* **5**, 183 (1961); R. W. Keyes and R. Landauer, *ibid.* **14**, 152 (1970).
8. C. Bennett, *ibid.* **17**, 525 (1973).
9. K. K. Likharev, *Int. J. Theor. Phys.* **21**, 311 (1982).
10. _____ and A. N. Korotkov, in *Abstracts of the Fourth International Workshop on Computational Electronics*, Tempe, AZ, 30 October to 5 November 1995, p. 5.
11. D. V. Averin and K. K. Likharev, in *Mesoscopic Phenomena in Solids*, B. L. Altshuler, P. A. Lee, R. A. Webb, Eds. (Elsevier, Amsterdam, 1991), pp. 173–271.
12. A. N. Korotkov and K. K. Likharev, report presented at the *International Conference on Quantum Devices and Circuits*, Alexandria, Egypt, 4 to 8 June 1996.
13. Our discussion of entropy transfer serves only as an interpretation of our quantitative result for the energy dissipation, rather than its basis.
14. D. V. Averin and A. N. Korotkov, *J. Low Temp. Phys.* **80**, 173 (1990); M. Kastner, *Rev. Mod. Phys.* **64**, 849 (1992).

15. We thank D. V. Averin and T. Usuki for useful discussions. Supported in part by Office of Naval Research grant N00014-93-1-0880 and Air Force Office of Scientific Research grant F49620-95-1-0044.

29 February 1996; accepted 17 June 1996

"Tubules-Within-a-Tubule" Hierarchical Order of Mesoporous Molecular Sieves in MCM-41

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The recently discovered mesoporous aluminosilicate MCM-41 consists of hexagonal arrays of nanometer-sized cylindrical pores. It is shown that this material can be synthesized by cooperative condensation of silicate and cylindrical cationic micelles. Careful control of the surfactant-water content and the rate of condensation of silica at high alkalinity resulted in hollow tubules 0.3 to 3 micrometers in diameter. The wall of the tubules consisted of coaxial cylindrical pores, nanometers in size, that are characteristic of those of MCM-41. The formation of this higher order structure may take place through a liquid crystal phase transformation mechanism involving an anisotropic membrane-to-tubule phase change. The hierarchical organization of this "tubules-within-a-tubule" particle texture is similar to that of the frustules of marine diatoms.

In the formation of mesoporous M41S family molecular sieves (*1*, *2*), cooperative formation of the surfactant phase is critical in determining the mesostructure (*2*, *3*). By varying the surfactant/silicate ratio, one can form hexagonal, cubic, or lamellar structures as the surfactant/silicate ratio increases (*2*, *4*). This is parallel to the known phase behavior in simple water/surfactant systems for cationic (*5*) and anionic (*6*) surfactants, where increasing surfactant concentration will usually make the following transformation: micellar solution L1 → hexagonal H1 → intermediate I → lamellar Lα (*5*). According to the balance of free energy between hydrophilic and hydrophobic groups, this transformation can also be brought about by decreasing the repulsion in the head group of the surfactant molecule (*6*).

For a complex mixture of surfactant and silicates, the liquid crystal structures formed are highly sensitive to the conditions of the solution. Various controllable factors, such as temperature, alkalinity, and the addition of counterions and alcohols, can induce mesoscopic structural change by modifying the rigidity and curvature of the interfaces (*7*–*11*). For the synthesis of MCM-41, when the structure is soft and before extensive polymerization of silicates, higher order organization may be thus controlled and formed. Here we report that solvent-separated multilayers of periodic hexagonal MCM-41 silicates can be formed and further bent into hollow microtubules (micrometer size) with the nanochannels forming the walls of these tubules. The resulting cylindrical silica has a hierarchical order of tubules within a tubule.

Surfactant and silicate were mixed in

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