QUANTUM-DOT ARRAYS: SIMULATION RESULTS TOWARD ANALOG COMPUTING

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ABSTRACT

Arrays of quantum dots (QD) produce bi-stable and multi-stable robust behavior, which can be harnessed for unconventional, yet powerful computing. In this paper, we propose a novel approach to signal pattern analysis using a two-dimensional array of QD, based on the formal analogy between the free energies of the QD array and a Hopfield neural network. Photon-assisted tunneling in the QD array enables realistic emulation of the plasticity of neural synapses. Simulation results illustrate the feasibility of the approach.

INTRODUCTION

Recent developments in nanoscale science and technology have opened exciting opportunities for revolutionary advances in nanoscale computing, communication, detection, and sensing. Fully exploiting this emerging potential requires a deep understanding of the complex dynamics and properties of small arrays of quantum structures, including quantum dots (QD), ultra small Josephson junctions, QD lasers, and others. Such arrays are known to produce robust bi-stable and multi-stable behavior, which can be harnessed for unconventional, yet powerful computing. The purpose of this paper is to address the issue of complex information processing by QD arrays. In particular, we are interested in demonstrating a capability for pattern classification using neuromorphic algorithms. The reader is referred to a companion paper [1] in this volume for a report of experimental progress toward this goal.

NEUROMORPHIC ALGORITHMS FOR COMPLEX INFORMATION PROCESSING

QD nanoelectronic and molecular electronic devices represent a promising hardware technology that offers both conceptual opportunities and engineering challenges for complex information processing applications (for example, see Ref. [2-5]). One such application, namely pattern recognition, is of considerable interest to the development of modern intelligent systems and will be considered here. The proven ability of neuromorphic algorithms to deal with uncertain information and to interact with dynamic environments is providing a strong incentive to explore the feasibility of implementing pattern recognition algorithms on nanoscale electronic devices.

Artificial neural networks are adaptive systems that process information by means of their response to discrete or continuous input [6]. Neural networks can provide practical solutions to a variety of artificial intelligence problems, including pattern recognition [7], autonomous knowledge acquisition from observations of correlated activities [8], real-time control of complex systems [9], and fast adaptive optimization [10]. At the heart of such advances lies the development of efficient computational methodologies for "learning" [11]. The development of neural learning algorithms has generally been based upon the minimization of an energy-like neuromorphic error function or functional [12].

Roychowdhury and his collaborators were the first to propose the implementation of neural networks in terms of QD arrays [13]. In their *Gedankenexperiment,* a generic array of nanometer-sized metallic islands would be deposited on a resonant tunneling diode. The Roychowdhury team showed that the evolution of an initial charge distribution toward a stable final equilibrium distribution can be given a neuromorphic interpretation and that this property emerges purely as a result of the discreteness of the electronic charge [14]. There are some shortcomings in their proposal. The most notable is the assumption that all inter-island capacitance could be modified arbitrarily, but offered no mechanism to achieve this essential property. Even though their paradigm would allow some elementary form of combinatorial optimization, Roychowdhury's proposal could not be used for neural learning needed in pattern recognition.

There is a formal similarity between the dynamics of neural networks and that of QD arrays that the proposal from [13] readily identified. In the latter, the electrostatic free energy characterized by a charge distribution of individual *excess* electrons in a QD array can be lowered in terms of quantum tunneling events. For neural networks, on the other hand, Hopfield has shown that the stable states of the network are the local minima of a bounded Lyapunov function of the net's output, parameterized by the synaptic interconnection weights. A careful analysis, however, reveals that this formal similarity is not sufficient for implementing learning algorithms for pattern recognition. By comparing the leading terms of the free energy (see Eq. (2) below), i.e., $\frac{1}{2}\vec{Q}^T \underline{C}^{-1}\vec{Q}$ and the Lyapunov function in a Hopfield network, i.e., $L(x,\underline{W}) = -\frac{1}{2}x^T \underline{W}\, x$, we see that the inverse of the augmented capacitance matrix would have to play the role of the synaptic matrix. However, the capacitance is fixed, and cannot be modified after device fabrication. An alternative approach for controlling the dynamics of the system has to be found. In principle, one could manipulate the free energy of the array via capacitive gating of each QD. However, for an array of quantum dots 1-to-2 nm in size, which is necessary for room temperature operation, we are not aware of technology capable of implementing such gating on an individual basis.

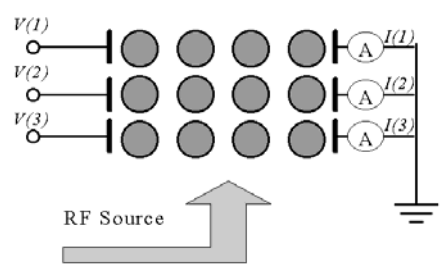

FIGURE1. Two-dimensional QD array showing voltages as input channels and currents as outputs.

Studies of the dynamics of arrays of QD in the presence of time-dependent excitations (e.g., RF signal [15,16]) reveal a rich structure of dynamical behaviors that offers a tremendous potential for performing the flexibility we need. In particular, a team led by Oosterkamp has recently made available an extensive survey of experiments and methods for photon-assisted tunneling in QD [17]. In the absence of a time-dependent field, current flows through a quantum dot via tunneling when an unoccupied internal energy state is aligned to the Fermi energy of the leads. However, as pointed out by Oosterkamp *et al.,* following seminal work by Likharev *et al.*, if a time-varying AC voltage $A_0 \cos(2\pi\omega t)$ is applied, inelastic tunnel events are induced when electrons

exchange photons of energy $\hbar\nu$ with the oscillating field. Tien and Gordon first described theoretically this phenomenon of multiphoton-assisted tunneling [18] (see Eq. (8) below).

We consider the transport voltage V as the input variable and the current I as the output function in designing the neuromorphic computation. For a two-dimensional QD array with M input and M output nodes, we can readily generalize the description of single-electron tunneling, given below, to consider M input voltages V_m and M output currents $I_m(V_m, A_0, \nu)$, $m = 1, 2, \ldots, M$ (see Fig. 1) . This vector function, $\overline{I_M}$, is controllable through the parameters of the external, alternating field, i.e., the field amplitude A_0 and frequency ν, by minimizing the error function E, defined over a numberof L training patterns as the squared difference between the l-th observed current, I_M^l ,

and the target currents, I_M^{l*} ,

$$E \equiv \frac{1}{L}\sum_{l=1}^{L}\left[I_M^l\left(V_M, A_0, \nu\right) - I_M^{l*}\right]^2 . \tag{1}$$

For convenience, vector dimensions are explicitly indicated as subscripts. If additional controls are necessary, then a polychromatic AC field may be considered for the global control, rather than a monochromatic field. In the following section, we demonstrate the modulation via interaction with an external, oscillatory field of the electric current as a function of the applied voltage through a QD array. This is the essential capability necessary for our approach to neuromorphic pattern-recognition in QD arrays.

SINGLE-ELECTRON TUNNELING IN A 1-D QUANTUM-DOT ARRAY

Consider a one-dimensional array of N tunnel junctions constructed from metallic source and drain electrodes weakly coupled to a linear array of N - 1 metal clusters. The "orthodox theory" of single-electron tunneling [2] is very successful in describing the charge transport through arrays of *low-conductance (high resistance)* tunnel junctions under small, but finite, bias voltage. The vector $\vec{n}$ defines the state of our system, $\vec{n} \equiv (n_1, \cdots, n_i, \cdots, n_{N-1})$, where n_i is the number of *excess* electrons accommodated by the ith quantum dot. The Gibbs free energy $E(\vec{n}, V)$ describing the electrostatic energy of the array of quantum dots and its interaction with the external voltage is

$$E\left(\vec{n}, V\right) = \frac{1}{2}\vec{Q}^T \underline{C}^{-1}\vec{Q} - V_s Q_s - V_d Q_d \tag{2}$$

where $C_{ij} = C_{ji}$ is the mutual capacitance between conductors i and j, and ϕ_i is the electrical potential of cluster i measured with respect to the substrate. The source and drain electrodes are enumerated as $i = 0$ and $i = N$, respectively. The source potential is $\phi_0 = V_s = V/2$, and the drain potential is $\phi_N = V_d = -V/2$. V is the transport voltage across the array. In writing Eq. (2) a matrix notation is used, i.e., $\vec{Q} = \underline{C}\vec{\phi}$, where generalized capacitance matrix elements and an augmented charged vector are defined.

In describing the electron transport through the array, we adopt the standard approximations of the "orthodox theory" approach, i.e., we neglect the effects of co-tunneling, and consider only single-electron tunneling between nearest neighbors in the array. That is, the final state $\vec{m}$ of the tunneling differs from the initial state $\vec{n}$ by the transfer of a single electron though the kth junction, e.g., $\vec{m} = \vec{n} \pm \Delta\hat{u}_k$, where $\Delta\hat{u}_k \equiv \hat{u}_k - \hat{u}_{k-1}$ and $\hat{u}_k$ is a unit vector for the kth quantum dot. The ± sign gives the direction of tunneling through the junction. If the transition rates are sufficiently small, one can perform a calculation using Fermi's Golden Rule to obtain [2]

$$\Gamma_k^{\pm}(\vec{n},V)=\Gamma_k^{\pm}\left(\Delta E_k^{\pm}(\vec{n},V)\right)=\frac{-\Delta E_k^{\pm}}{e^2R_k}\left[1-\exp\left(\frac{\Delta E_k^{\pm}}{k_BT}\right)\right]^{-1} \tag{3}$$

where $\Delta E_k^{\pm}(\vec{n},V)\equiv E(\vec{n}\pm\Delta u_k,V)-E(\vec{n},V)$ is the change in the free energy of the system due to tunneling, R_k is the effective resistance of the tunnel junction, $e>0$ is the fundamental unit of charge, and the thermal energy is k_BT. The master equation describing the time evolution of the probability $P(\vec{n},t)$ of finding the circuit in the state $\vec{n}$ is

$$\frac{dP(\vec{n},t)}{dt}=\sum_k\left[\Gamma_{k-1}^{+}(\vec{n}-\Delta\hat{u}_{k-1})P(\vec{n}-\Delta\hat{u}_{k-1},t)+\Gamma_k^{-}(\vec{n}+\Delta\hat{u}_k)P(\vec{n}+\Delta\hat{u}_k,t)\right]-\sum_{k=1}^{N}\left[\Gamma_k^{+}(\vec{n})+\Gamma_k^{-}(\vec{n})\right]P(\vec{n},t) \tag{4}$$

Practical approaches to solving the master equation are described in Refs. [3-5], and software to solve these equations is available in the public domain [19]. Given the solution of Eq. (4), the average tunneling current is given by computing the net flow through any junction k in the array:

$$I(V)=I_k(V)=e\sum_{\vec{n}}P(\vec{n})\left[\Gamma_k^{+}(\vec{n},V)-\Gamma_k^{-}(\vec{n},V)\right], \tag{5}$$

where $P(\vec{n})$ is the time average of $P(\vec{n},t)$.

Multiphoton-assisted tunneling. Tien and Gordon first described theoretically the phenomenon of multiphoton-assisted tunneling (PAT) [18] for electron transport in the presence of a time-varying AC voltage $A_0\cos(2\pi\omega t)$. The tunneling rate $\bar{\Gamma}$ through each barrier in the presence of an electromagnetic excitation in terms of the rates without the external AC field,

$$\bar{\Gamma}_k^{\pm}(\vec{n},V,A_0,\nu)=\sum_{\alpha=-\infty}^{\infty}J_\alpha\left(\frac{eA_0}{\hbar\nu}\right)\Gamma_k^{\pm}(\Delta E_k^{\pm}+\alpha\hbar\nu) \tag{6}$$

where J_α denotes the Bessel function of the first kind and α denoting the number of photons exchanged. The master equation is generalized to account for PAT processes by substituting the rates given by Eq. (6) into Eq. (4). Then, the current through the 1-D QD array becomes a function of the amplitude A_0 and frequency ν of the AC field, in addition to the transport voltage V,

$$I(V,A_0,\nu)=e\sum_{\vec{n}}P(\vec{n})\left[\bar{\Gamma}_k^{+}(\vec{n},V,A_0,\nu)-\bar{\Gamma}_k^{-}(\vec{n},V,A_0,\nu)\right]. \tag{7}$$

We have numerically solved Eq. (7) applying well-known Monte-Carlo approaches [3,4,5] by modifying the public domain software [19] to include the PAT rates from Eq.(6). Results shown in Fig. (2), demonstrate that the current through a 1D QD array with 3 QDs can be effectively modulated by the applied frequency of external oscillatory field. These simulations confirm that PAT can be used to control the charge transport through QD arrays in a manner that preserve the desired non-linear current-voltage relations (e.g., Coulomb blockade, Coulomb staircase).

High-conductance tunnel junctions. From a practical point of view, large arrays have advantages, e.g., good electrical isolation of the inner QD from the environment. At the same time, increasing the number of junctions in the array, increases its total resistance. This makes it attractive to consider high-conductance tunnel junctions, in contrast to the low-conductance junctions considered in the previous section. Theoretical work on this topic has demonstrated that under certain conditions, the non-linear current-voltage behavior we desire (e.g., Coulomb-blockade, Coulomb staircase) survives into the high-conductance regime [20].

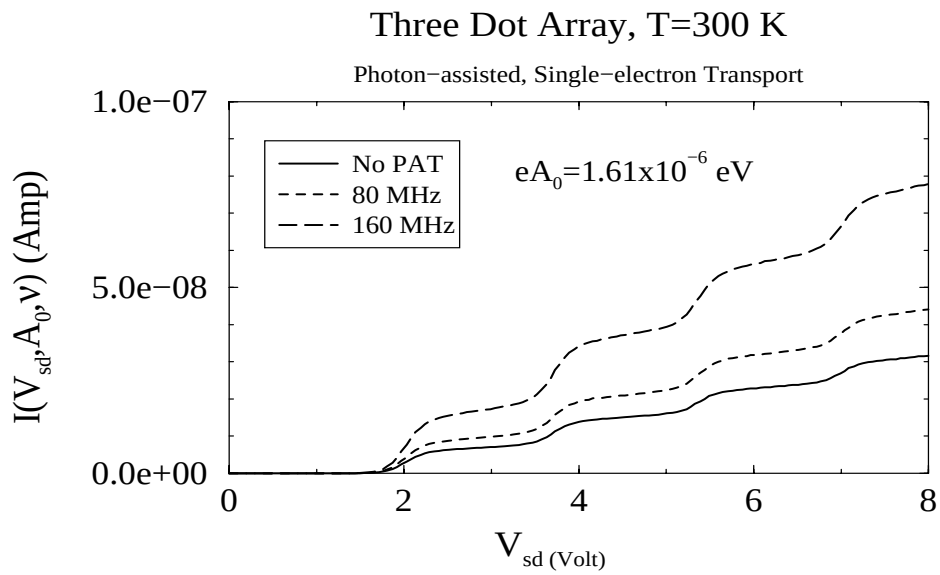

FIGURE 2. Current-voltage characteristics through a 1-D QD array with the current modulated by multiphoton-assisted tunneling.

Consider a one-dimensional array of N quantum dots with high-conductance tunnel junctions. Their dynamics is described by the Langevin equations [20]:

$$C_j \frac{\hbar}{2e}\ddot{\varphi}_j + \frac{1}{R_j}\frac{\hbar}{2e}\dot{\varphi}_j = \dot{q} + \tilde{\xi}_j \qquad j = 1,...N \tag{8}$$

$$V_x = \dot{q}\, R_s - \xi_s\, R_s + \sum_{k=1}^{N} \dot{\varphi}_k$$

Here $\varphi_j(t)$ is the junction phase, defined such that

$$\frac{\hbar}{2e}\dot{\varphi}_j(t) = V_j \tag{9}$$

is the voltage drop across junction j. The external voltage is denoted by V_x. With each junction, there is an associated shot noise

$$\tilde{\xi}_j = a_j \cos(\frac{\varphi_j}{2}) + b_j \sin(\frac{\varphi_j}{2}), \tag{10}$$

where a_j and b_j are correlated Gaussian random variables with specific properties. R_s and ξ_s are, respectively, the resistance of the electromagnetic environment and a noise-like local perturbation to the current, $\dot{q}$.

The dimensionless equations for the array dynamics are obtained by combining Eqs. (8) and (9), and by eliminating the circuit current. Moreover, it is common to express the phases in scaled time units, scaled by a frequency parameter ω. We obtain

$$\ddot{\varphi}_j + \gamma\dot{\varphi}_j + \beta\sum_{k=1}^{N}\dot{\varphi}_k = v_x + \frac{R_s}{V_0}\xi_j \tag{11}$$

where V_0 is a normalization voltage, and

$$v_x = V_x / V_0 \,;\; \gamma = 1/(\omega\tau) \,;\; \beta = 1/(\omega\tau_s) \,;\; \tau = RC \,;\; \tau_s = R_s C \,; \text{ and } \omega = \sqrt{\frac{2e}{\hbar}\frac{V_0}{\tau_s}} \,.$$

In deriving Eq.(11), we have assumed that ξ_s is zero, and that all resistances are equal to *R*, and all capacitances are equal to *C*. The procedure used to calculate the averaged current $< i >$ in terms of the dimensionless external voltage v_x is as follows. Let

$$\mathrm{Q}_j^{\varphi} = \sum_{n=N_i}^{N} \dot{\varphi}_j(t_n) \qquad \text{and} \qquad \mathrm{Q}_j^{\xi} = \sum_{n=N_i}^{N} \xi_j(t_n).$$

Then,

$$< i > (v_x) = \frac{1}{N}\sum_{j=1}^{N} < i >_j = \frac{1}{N}\sum_j (\gamma Q_j^{\varphi} - \frac{R_s}{V_0} Q_j^{\xi}) \,.$$

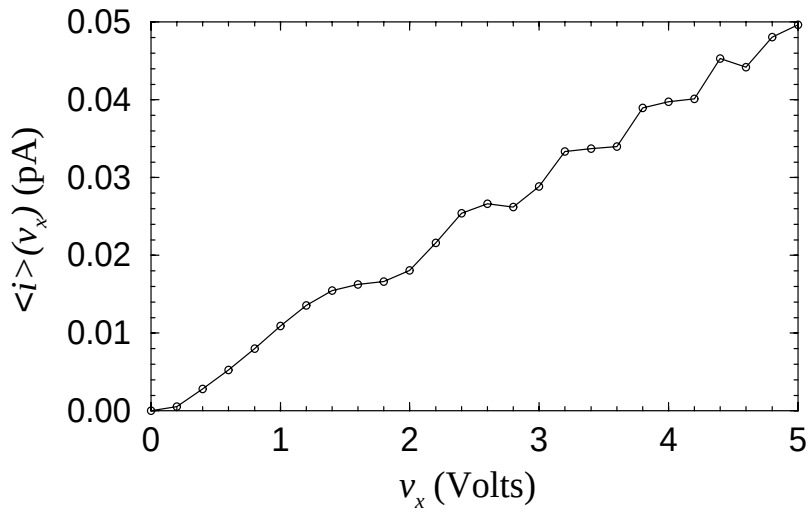

FIGURE 3. Current-voltage relations computed by the Langevin Equation approach demonstrating the Coulomb-blockade and Coulomb-staircase phenomena for a 1-D array of low-conductance tunnel junctions.

SUMMARY AND CONCLUSIONS

In this paper, we have explored an opportunity for implementing neuromorphic algorithms for pattern recognition in QD arrays of sufficiently close so that transport through the array occurs via single-electron tunneling. Previous work on this topic is discussed, based on the formal analogy between the Lyapunov function of a neural

network and the electrostatic free energy of a quantum-dot array. While attractive, it is practically difficult to leverage this analogy for pattern recognition because of one's inability to modify the capacitance of the QD array after fabrication of the device. One possibility around this obstacle is to interface a gate electrode to each (or to many) QDs in the array. This also has tremendous technical difficulties for QD of a size appropriate for room-temperature operation (~ 1 nm). An alternative approach is to modulate the current-voltage relations of the QD array by interaction with an oscillatory applied field. We have presented simulation results that demonstrate that various parameters of the field (i.e., frequencies and amplitudes within realistic ranges) may be used to modulate the current, and therefore utilized as control parameters for the neuromorphic pattern recognition algorithms. In this manner, rather than insisting on using external controls local in space (which are not practical), we choose external controls that are localized in a reciprocal space (e.g., frequency space).

For simplicity in this paper, we have neglected this discreteness in the density of electronic states in the cluster resulting from their small size. However, as discussed in our companion paper [1], we are interested in nanometer-sized metal clusters in which the Coulomb blockade of conductance may be observed at room temperature. In such nanocluster systems, the energy gap between the highest-occupied and lowest-unoccupied orbitals can be as large as 0.5 eV. For a quantitative description of such systems, one should not neglect the discreteness of the density of electronic states, as these features will introduce new transport channels producing new features into the current-voltage relationship. The qualitative result presented here of the modulation of the current by photon-assisted tunneling is expected to be unaffected by the simplifications employed here.

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REFERENCES

1. T. THUNDAT, K. STEVENSON, L. MAYA, M. GOVINDARAJAN, J. C.WELLS, and J. BARHEN, "Site-Specific Attachment of Nanoparticles to DNA Templates", proceedings of this symposium.

2. K. K. LIKHAREV, "Single Electron Devices and their Applications", *Proc. IEEE*, **87**(4), 606-632 (1999).

3. L. R. C. FONSECA, A. N. KOROTKOV, K. K. LIKHAREV, and A. A. ODINTSOV, "A Numerical Study of the Dynamics and Statistics of Single-Electron Systems", *J. Appl. Phys.* **78**, 3238 (1995).

4. S. FÖLLING, Ö. TÜREL, AND K. LIKHAREV, "Single-Electron Latching Switches as Nanoscale Synapses", in: Proc. of Int. Joint Conf. on Neural Networks (Washington, DC, July 2001), Int. Neural Network Society, Mount Royal, NY, 2001, pp. 216-221.

5. A. S. CORDAN and A. GOLTZENE., "Optimization of the Master Equation Set for a Multidot Tunnel Structure", *Eur. Phys. J AP* **7**, 137 (1999).

6. M. HASSOUN, *Fundamentals of Artificial Neural Networks*, MIT Press (1995).

7. M. BISHOP, *Neural Networks for Pattern Recognition*, Oxford University Press (1997).

8. M. BECKERMAN, *Adaptive Cooperative Systems*, Wiley Interscience (1997).

9. D. WHITE and D. SOFGE, *Handbook of Intelligent Control: Neural, Fuzzy, and Adaptive Approaches*, Van Nostrand Reinhold (1992).

10. A. CICHOCKI and R. UNBENHAUEN, *Neural Networks for Optimization and Signal Processing*, Wiley (1993).

11. P. MARS, J. CHEN, and R. NAMBIAR, *Learning Algorithms*, CRC Press (1996).

12. Y. CHAUVIN and D. RUMELHART, *Backpropagation: Theory, Architectures, and Applications*, Lawrence Erlbaum (1995).

13. V. ROYCHOWDHURY, D. JANES, S. BANDYOPADHYAY, and X. WANG, "Collective Computational Activity in Self-Assembled Arrays of Quantum Dots: Novel Neuromorphic Architectures for Nanoelectronics", *IEEE Trans. Electron. Devices* **42**(10), 1688-1698 (1996).

14. S. BANDYOPADHYAY and V. ROYCHOUDHURY, "Computational Paradigms in Nanoelectronics: Quantum Coupled Single Electron Logic and Neuromorphic Networks", *Jap. Jour. Applied Phys.*, **35**(6), 3350-3362 (1996).

15. L. P. KOUWENHOVEN A. JOHNSON, N. VAN DER VAART, C. HARMANS, and C. FOXON, "Quantized Current in a Quantum-Dot Turnstile Using Oscillating Tunnel Barriers", *Phys. Rev. Lett*. **67**, 1626-1629 (1991).

16. M. N. WYBOURNE, L. CLARKE, M. YAN, S. CAI, L. BROWN, J. HUTCHISON, and J. KEANA, "Coulomb-Blockade Dominated Transport in Patterned Gold-Cluster Structures", *Jap. Jour. Appl. Phys*., **36**, 7796 (1997).

17. T. OOSTERKAMP, W. VAN DER WIEL, S. DeFRANCESCHI, C. HARMANS, and L. KOUWENHOVEN, "Photon Assisted Tunneling in Quantum Dots", *arXiv:cond-mat/9904359*, LANL (26 April 1999).

18. P. K. TIEN and J. P. GORDON, "Multiphoton Process Observed in the Interaction of Microwave Fields with the Tunneling between Superconductor Films," *Phys. Rev.* **129**, 647 (1963).

19. MOSES 1.0, "Monte-Carlo Single-Electron Simulator", Copyright 1995, RUBY HUI CHEN, with contributions from A. K. MATSUOKA, A. N. KOROTKOV, B. HARRIS, P. SHEVCHENKO, and K. K. LIKHAREV.

20. SH. FARHANFAR, R. S. POIKOLANIEN, J. P. PEKOLA, D. S. GOLUBEV, and A.D ZAIKIN, "Coulomb Blockade in One-Dimensional Arrays of High-Conductance Tunnel Junctions", *Phys. Rev. B* **63**, 075309 (2001).