Coulomb blockade threshold in inhomogeneous one-dimensional arrays of tunnel junctions

J. A. Melsen
Instituut-Lorentz, University of Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

Ulrik Hanke, H.-O. Müller,* and K.-A. Chao*
Department of Physics and Mathematics, Norwegian Institute of Technology, University of Trondheim, 7034 Trondheim, Norway
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A general expression is given for the change in free energy when a charge tunnels through a junction in a one-dimensional array of N metallic islands with arbitrary capacitances and arbitrary background charges. This is used to obtain expressions for the (average) threshold voltage of the Coulomb blockade for a few characteristic geometries. We find that including random background charges has a large effect on the N dependence of the threshold voltage: In an array with identical junction capacitances C and gate capacitances C_g, the threshold voltage, averaged over the background charge, is proportional to N^a, where a crosses over from $\frac{1}{2}$ to 1 when N becomes larger than $2.5\sqrt{C/C_g}$.
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I. INTRODUCTION

Since the pioneering work by Gorter in 1951,[1] single charge tunneling effects have been extensively studied in various kinds of geometries.[2] Research on single electronics has led to potential applications in, e.g., current standards,[3,4] ultradense integrated digital electronics,[5] thermometry,[6,7] and room-temperature memory.[8] In many of these applications, tunneling occurs through a large number of junctions in series. Most theoretical work has assumed homogeneous arrays.[9–13] The problem is that the number of available states at a finite current rapidly increases with the circuit size, so that one either restricts the analysis to homogeneous arrays or adopts a numerical approach.[14] Using modern techniques, it is possible to fabricate arrays of metallic islands separated by tunnel junctions with almost uniform capacitances. It is however very difficult to avoid nonuniform background charges on the islands. This is relevant, since the charging energy is very sensitive to the background charge.

The aim of this paper is to provide results for *inhomogeneous* one-dimensional arrays of metallic islands. The inhomogeneity can be both in the junction capacitances and in the background charges on the islands in the array. In particular, we study the threshold voltage for charge transport. The results obtained are exact within the classical (orthodox) model of single-electron tunneling,[15] which is accurate when quantum size effects and macroscopic quantum tunneling effects may be ignored.

Using a general expression for the inverse capacitance matrix, we calculate in Sec. II the change in the free energy of an N junction array due to an arbitrary tunneling event. In Sec. III, we focus on the threshold voltage for transport V_t, which is an observable quantity. We find that inhomogeneity of the junction capacitances C has a small effect on the threshold voltage in large arrays: The expectation value as $N\rightarrow\infty$ for the threshold voltage of an array without gate coupling (gate capacitance $C_g=0$ for each junction) and without background charges is $\langle V_t\rangle=\frac{1}{2}Ne\langle C^{-1}\rangle$, with $\langle C^{-1}\rangle$ being typically not much different from $1/\langle C\rangle$. However, as we show in Sec. IV, a random variation in background charges may change the threshold voltage considerably: In a short array with weak gate coupling ($N^2C_g/6.25C<1$) and random charges on all N islands, we find $\langle V_t\rangle\propto\sqrt{N}$. In a long array with strong gate coupling ($N^2C_g/6.25C\gg 1$, but still $C_g\ll C$), we find $\langle V_t\rangle\propto N$. We compare our results with experiments.[16]

II. FREE ENERGY

The system under consideration is shown schematically in Fig. 1. Within the orthodox model, the state of the system is described by the numbers n_i of electrons on the ith island, which we combine in a vector: $\vec{n}\equiv(n_1,n_2,\ldots,n_{N-1})$. The tunneling rate, $\Gamma_k(\vec{n})$, corresponding to a single electron tunneling from island $k-1$ to island k is given by[2]

$$\Gamma_k(\vec{n})=\frac{\Delta G_k(\vec{n})}{e^2R_k\{1-\exp[-\Delta G_k(\vec{n})/k_{\mathrm{B}}T]\}}. \qquad (2.1)$$

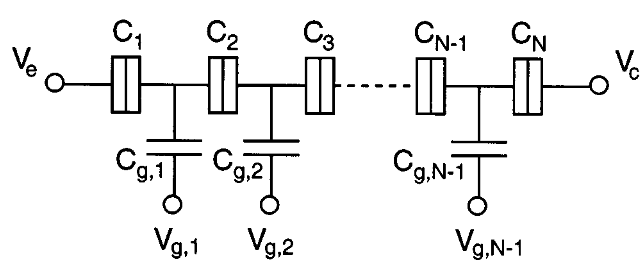

FIG. 1. Schematic diagram of a one-dimensional array of N tunnel junctions. Island i is coupled to island $i+1$ by a tunnel barrier with capacitance C_{i+1}, and to a gate electrode by an insulating barrier with capacitance $C_{g,i}$. The capacitance C_1 (C_N) denotes the coupling of the first (last) island to the emitter (collector) electrode.

Here R_k is the resistance of the kth tunnel junction and $\Delta G_k(\vec{n})$ is defined as the difference in free energy of the final and initial states. The free energy comprises the electrostatic energies of the charged capacitors in the system, as well as the potential energies of all electrodes:[9]

$$G(\vec{n}) = \frac{1}{2}\sum_{i=1}^{N-1} C_{g,i}(\phi_i - V_{g,i})^2 + \frac{1}{2}\sum_{i=1}^{N} C_i(\phi_i - \phi_{i-1})^2 - V_e Q_e - V_c Q_c - \sum_{i=1}^{N-1} V_{g,i} Q_{g,i}. \quad (2.2)$$

We denote by ϕ_i the electrochemical potential of island i ($\phi_0 \equiv V_e$ and $\phi_N \equiv V_c$), and by Q_e, Q_c, and $Q_{g,i}$ the charges on the emitter, collector, and gates, respectively:

$$Q_e = C_1(V_e - \phi_1) + e n_e, \quad (2.3a)$$

$$Q_c = C_N(V_c - \phi_{N-1}) + e n_c, \quad (2.3b)$$

$$Q_{q,i} = C_{g,i}(V_{g,i} - \phi_i). \quad (2.3c)$$

Here n_e (n_c) is the number of electrons that has tunneled from the emitter (collector) electrode through the first (last) capacitor.

The difficulty in determining the energy difference $\Delta G_k(\vec{n})$ lies in the determination of the electrochemical potentials $\vec{\phi} \equiv (\phi_1, \phi_2, \ldots, \phi_{N-1})$. They follow from the condition that the total capacitive charge on each island i equals $e n_i$ plus a background charge $Q_{0,i}$:

$$C_{g,i}(\phi_i - V_{g,i}) + C_i(\phi_i - \phi_{i-1}) + C_{i+1}(\phi_i - \phi_{i+1}) = e n_i + Q_{0,i}, \quad i = 1,2, \ldots, N-1. \quad (2.4)$$

The background charge $Q_{0,i} \in (-e/2, e/2)$ is due to incompletely screened charges in the environment of the island. Equation (2.4) can be written in matrix form as $\mathbf{C}\vec{\phi} = \vec{Q'}$, with

$$\boldsymbol{C}_{ij} = \delta_{i,j}(C_i + C_{i+1} + C_{g,i}) - \delta_{i+1,j} C_j - \delta_{i,j+1} C_i, \quad (2.5a)$$

$$Q'_i = e n_i + Q_{0,i} + C_{g,i} V_{g,i} + \delta_{i,1} C_1 V_e + \delta_{i,N-1} C_N V_c. \quad (2.5b)$$

The capacitance matrix $\boldsymbol{C}$ can be inverted exactly. The elements $R_{i,j}$ of the inverse capacitance matrix $\boldsymbol{R} = \boldsymbol{C}^{-1}$ are given by

$$R_{i,j} = C_{i+1} C_{i+2} \cdots C_j D_{i-1} \widetilde{D}_{j+1} D_{N-1}^{-1}, \quad i \leqslant j,$$
$$R_{j,i} = R_{i,j}. \quad (2.6)$$

Here we have introduced the subdeterminants D_i ($\widetilde{D}_{N-i}$) of the upper left (lower right) capacitance submatrix of dimension i. These can be found recursively from

$$D_i = (C_i + C_{i+1} + C_{g,i}) D_{i-1} - C_i^2 D_{i-2}, \quad (2.7a)$$

$$\widetilde{D}_i = (C_i + C_{i+1} + C_{g,i}) \widetilde{D}_{i+1} - C_{i+1}^2 \widetilde{D}_{i+2}, \quad (2.7b)$$

$$D_0 \equiv \widetilde{D}_N \equiv 1. \quad (2.7c)$$

For a homogeneous array with identical capacitances, $C_1 = C_2 = \ldots = C_N$ and $C_{g,1} = C_{g,2} = \ldots = C_{g,N-1}$, we recover the inverse capacitance matrix of Ref. 12.

We now derive a general expression for the difference in free energy $\Delta G_k(\vec{n})$ when an electron tunnels from island $k-1$ to island k. Applying Eq. (2.7) and making use of the orthogonality relation

$$(C_i + C_{i+1} + C_{g,i}) R_{i,j} = C_i R_{i-1,j} + C_{i+1} R_{i+1,j} + \delta_{i,j}, \quad (2.8)$$

we find that $\Delta G_k(\vec{n})$ takes the form

$$\Delta G_k(\vec{n}) = -\frac{e^2}{2}(R_{k-1,k-1} + R_{k,k} - R_{k-1,k} - R_{k,k-1}) + e\sum_{i=1}^{N-1} Q_i (R_{i,k-1} - R_{i,k}) + e(V_e - V_{g,1}) A_{1,k} + e\sum_{i=2}^{N-1} (V_{g,i-1} - V_{g,i}) A_{i,k} + e(V_{g,N-1} - V_c) A_{N,k}, \quad (2.9a)$$

$$A_{i,k} = C_i (R_{i-1,k} + R_{i,k-1} - R_{i-1,k-1} - R_{i,k}) + \delta_{i,k}. \quad (2.9b)$$

Here, $R_{i,N} = R_{0,i} = 0$ is implied, and $Q_i = e n_i + Q_{0,i}$.

Although we are now able to construct all relevant transition rates from expressions (2.6) and (2.9), the analytic evaluation of the current-voltage characteristic at arbitrary voltage remains a technically involved problem. The threshold voltage, however, is determined by a single transition rate and is therefore easier to evaluate. In the next two sections, we apply our results to this quantity for several characteristic geometries.

III. THRESHOLD VOLTAGE

Electron transport through a one-dimensional array is realized by a sequence of tunneling events through all junctions between the emitter and the collector (we refer to this as a tunneling sequence). At zero temperature, a specific tunneling sequence contributes to the conductance if the free energy difference of each tunneling event in the sequence is positive. The threshold voltage V_t of the Coulomb blockade is the smallest voltage at which a current can flow through the array at zero temperature. When $|V_e - V_c| < |V_t|$, there exists no conductive tunneling sequence. We first consider the simple case where the system is not gated ($C_{g,i} = 0$ for all i), and then discuss the turnstile configuration, i.e., an array which is coupled to a gate electrode via a single island: $C_{g,i} = C_g \delta_{i,n}$.

A. No gate coupling

In the absence of gate coupling, the determinants D and $\widetilde{D}$, following from Eq. (2.7), have a simple form. For convenience, we introduce the notation

$$S_k^l \equiv \sum_{i=k+1}^{l} \frac{1}{C_i}, \quad S^l \equiv S_0^l, \quad S_k \equiv S_k^N. \quad (3.1)$$

In terms of these quantities,

$$D_k=C_1C_2\cdots C_{k+1}S^{k+1}, \tag{3.2a}$$

$$\widetilde{D}_k=C_kC_{k+1}\cdots C_NS_{k-1}, \tag{3.2b}$$

$$R_{i,j}=S^iS_j/S^N, i\leqslant j. \tag{3.2c}$$

We further define $\vec{q}\equiv\vec{n}+\vec{q}_0$, $\vec{q}_0\equiv e^{-1}(Q_{0,1},Q_{0,2},\ldots,Q_{0,N-1})$. From the condition $\Delta G_k(\vec{q})=0$, we determine the threshold voltage $V_{t,k}(\vec{q})$ for tunneling through capacitance C_k at arbitrary occupation $\vec{q}$ of the array:

$$V_{t,k}(\vec{q})=\frac{e}{2}\left(S^N-\frac{1}{C_k}\right)-e\sum_{i=1}^{k-1}q_iS^i+e\sum_{i=k}^{N-1}q_iS_i. \tag{3.3}$$

The threshold voltage is determined as follows. For an initial charge state, we determine the minimal activation energy $eV_{t,k}(\vec{q})$ to allow a tunneling event in the array, as well as the corresponding final charge state. The final charge state becomes the initial state in the next step. The minimal activation energy for the new charge state and the corresponding final charge state are again determined, and this procedure is repeated until one electron has been transported from emitter to collector. The largest of the activation energies found equals eV_t. In the special case that all background charges are zero, one has

$$V_t=\tfrac{1}{2}e\left(\sum_{i=1}^{N}1/C_i-\text{Max}[1/C_1,1/C_2,\ldots,1/C_N]\right), \tag{3.4}$$

which is an extension of the result $V_t=\frac{1}{2}e\text{Min}[1/C_1,1/C_2]$ for a double junction.[17] For $N\rightarrow\infty$, V_t has a Gaussian distribution with average $\frac{1}{2}Ne\langle C^{-1}\rangle$ and variance $\text{Var}V_t=\frac{1}{4}Ne^2\,\text{Var}C^{-1}$.

B. Turnstile configuration

We next consider a turnstile configuration, i.e., an array with a single gate electrode coupled capacitively (capacitance C_g) to island n. The elements of the inverse capacitance matrix are then given by

$$R_{i,j}=(S^i+C_gS^nS_n^i)S_j(S^N+C_gS^nS_n)^{-1},\quad n\leqslant i\leqslant j,$$

$$R_{i,j}=S^iS_j(S^N+C_gS^nS_n)^{-1},\quad i\leqslant n\leqslant j,$$

$$R_{i,j}=S^i(S_j+C_gS_j^nS_n)(S^N+C_gS^nS_n)^{-1},\quad i\leqslant j\leqslant n,$$

$$R_{j,i}=R_{i,j}. \tag{3.5}$$

In order to determine the threshold voltage $V_{t,k}(\vec{q})$, we have to distinguish between $k\leqslant n$ and $k>n$. From Eqs. (2.9) and (3.5) we find that $V_{t,k}(\vec{q})$ now depends on the gate voltage V_g:[18]

$$V_{t,k}(\vec{q})=\frac{e}{2}\left(S'^N-\frac{1}{C'_k}\right)-e\sum_{i=1}^{k-1}q_iS'^i+e\sum_{i=k}^{N-1}q_iS'_i+C_g\times[V_g-\tfrac{1}{2}(V_e+V_c)]\begin{cases}S_n(1+\frac{1}{2}C_gS_n)^{-1}, & k\leqslant n\\ -S^n(1+\frac{1}{2}C_gS^n)^{-1}, & k>n,\end{cases} \tag{3.6}$$

where S' is defined as in Eq. (3.1) in terms of modified capacitances C':

$$C'_l=C_l(1+\tfrac{1}{2}C_gS_n)(1+C_gS_n)^{-1},\quad k\leqslant n,l\leqslant n,$$

$$C'_l=C_l(1+\tfrac{1}{2}C_gS_n),\quad k\leqslant n,l>n,$$

$$C'_l=C_l(1+\tfrac{1}{2}C_gS^n),\quad k>n,l\leqslant n,$$

$$C'_l=C_l(1+\tfrac{1}{2}C_gS^n)(1+C_gS^n)^{-1},\quad k>n,l>n. \tag{3.7}$$

IV. BACKGROUND CHARGE

The background charge in a single-electron tunneling device has a large influence on its properties. For example, by tuning the background charge in a double junction with one gate one can set the threshold voltage to any value between zero and $e/(2C+C_g)$. In this section, we investigate the effect of background charges on the threshold voltage of an array of tunnel junctions. For reasons of clarity, we choose identical junction capacitances in the following ($C_i=C$ for all i). We start by investigating an array with a nonzero background charge on a single island. We then give ensemble-averaged results for random background charges on all islands and compare with the experiments of Delsing *et al.*[16]

In the absence of gate coupling ($C_{g,i}=0$ for all i) and for a nonzero background charge $q_{0,m}=Q_{0,m}/e$ on island m, there are three initial tunneling events which may form the bottleneck for conduction: (i) transfer of an electron from the emitter to the first island (electron injection through junction $k=1$); (ii) tunneling through junction $k=m+1$ if $q_{0,m}>0$ or through junction $k=m$ if $q_{0,m}<0$ (electron-hole creation at island m); (iii) transfer from the last island to the collector (hole injection through junction $k=N$).

An analysis of the corresponding tunneling sequences results in the threshold voltage

$$V_t=\frac{e}{2C}\{N-1-2\text{Min}[mq_{0,m},(N-m)(1-q_{0,m})]\},\quad q_{0,m}\geqslant 0, \tag{4.1a}$$

$$V_t=\frac{e}{2C}\{N-1-2\text{Min}[m(1-|q_{0,m}|),(N-m)|q_{0,m}|]\},\quad q_{0,m}<0. \tag{4.1b}$$

For a uniform distribution of $q_{0,m}$ between $\pm\frac{1}{2}$ and a uniform distribution of m between 1 and $N-1$ its expectation value is $\langle V_t\rangle=(5N-7)e/12C$, with variance $\mathrm{Var}V_t=(e/2C)^2(N+1)(3N^2-5N+8)/180N$. The expectation value is slightly smaller than for a homogeneous array without background charges: $V_t=(N-1)e/2C$. In the limit $N\to\infty$ the root-mean-square deviation is $\mathrm{rms}V_t\propto Ne/C$, of the same order as the threshold voltage itself.

We next consider a one-dimensional array of equally gated islands ($C_i=C$, $C_{g,i}=C_g$ for all i). In Refs. 9 and 12 the charge transport in homogeneous arrays by solitonlike excitations was introduced. In terms of the soliton width $\lambda^{-1}=[2\,\mathrm{arsinh}\sqrt{C_g/4C}]^{-1}$ of Ref. 9, the threshold voltage for an electron tunneling through junction k is given by

$$V_{t,k}(\vec{q})=\frac{e}{2C}\Bigg(-2\sum_{i=1}^{k-1}(q_i+q_g)\sinh(i\lambda)\cosh[(N-k+\tfrac{1}{2})\lambda]+2\sum_{i=k}^{N-1}(q_i+q_g)\sinh[(N-i)\lambda]\cosh[(k-\tfrac{1}{2})\lambda]+\sinh[(N-\tfrac{1}{2})\lambda]-\cosh[(N-2k+1)\lambda]\sinh\frac{\lambda}{2}\Bigg)\times\left(\sinh\lambda\cosh\frac{N\lambda}{2}\cosh\frac{(N-2k+1)\lambda}{2}\right)^{-1}. \tag{4.2}$$

Here, the gate-induced charge $q_g\equiv C_g[V_g-\frac{1}{2}(V_e+V_c)]$ acts as an offset on the background charge. The average threshold voltage (averaged over the background charge) is therefore independent of V_g. For $N=2$, we find

$$\langle V_t\rangle=e/(4C+2C_g). \tag{4.3}$$

In the absence of background charges and for $q_g=0$, we find

$$V_t=\frac{e}{2C}\,\frac{\sinh[(N-1)\lambda/2]}{\cosh(N\lambda/2)\sinh(\lambda/2)}, \tag{4.4}$$

which approaches a constant value as $N\to\infty$, provided $\lambda\neq 0$, i.e., provided $C_g/C\neq 0$. In Fig. 2 we show the effect of random background charges on all islands in arrays of different lengths for several gate couplings, as calculated from Eq. (4.2). The averages are computed numerically by putting a random charge $q_{0,k}\in(-\frac{1}{2},\frac{1}{2})$ on each island k. The dependence of $\langle V_t\rangle$ on the array length differs drastically from the result (4.4) without background charges: Instead of a threshold voltage which exponentially approaches a constant value as $N\to\infty$, we find $\langle V_t\rangle\propto\sqrt{N}-1$ for small arrays, with a crossover to a linear N dependence for large arrays. For $C_g\ll C$, the array length N_c at which the crossover occurs is found to be 2.5 times the soliton width,

$$N_c\approx 2.5\sqrt{C/C_g}\approx 2.5\lambda^{-1}. \tag{4.5}$$

For $N<N_c$ the average threshold voltage is well described by an extrapolation of the result (4.3) for $N=2$:

$$\langle V_t^{<}\rangle=\frac{e}{4C+2C_g}\,\frac{\sqrt{N}-1}{\sqrt{2}-1}. \tag{4.6}$$

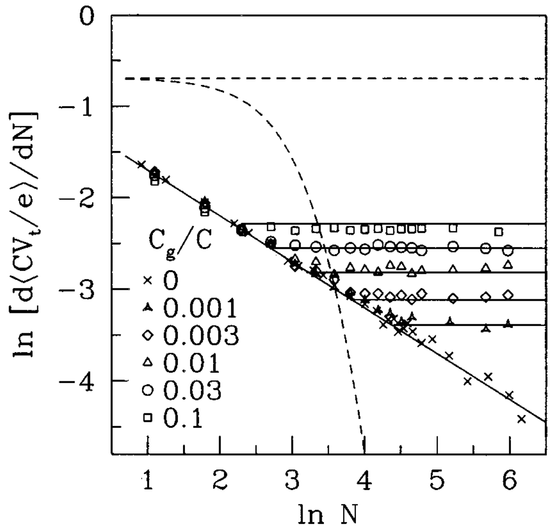

FIG. 2. Derivative of the average threshold voltage with respect to the array length N, for ensembles of arrays with identical capacitances ($C_i=C$ and $C_{g,i}=C_g$ for all i) and random background charges on all islands, calculated from Eq. (4.2). The average is determined numerically from ensembles of 10 000 samples for $N\leqslant 128$ and ensembles of 1000 samples for larger arrays. A crossover from $\langle V_t\rangle\propto N^{1/2}$ to $\langle V_t\rangle\propto N$ occurs at $N_c\approx 2.5\sqrt{C/C_g}$. Solid lines are the extrapolation formulas (4.6) and (4.7). The dashed curves are obtained from the result (4.4) for zero background charges and $C_g/C=0$ (upper curve) and $C_g/C=0.01$ (lower curve).

For $N>N_c$ we can describe the numerical data by

$$\langle V_t^{>}\rangle=\langle V_t^{<}\rangle_{N=N_c}+(N-N_c)\frac{d\langle V_t^{<}\rangle}{dN}\bigg|_{N=N_c}=\frac{e}{4C+2C_g}\,\frac{1}{\sqrt{2}-1}\left(\frac{N+N_c}{2\sqrt{N_c}}-1\right). \tag{4.7}$$

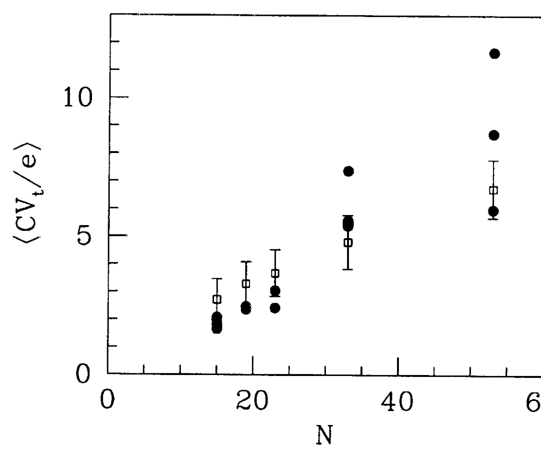

FIG. 3. Comparison of experimental threshold voltages (taken from Ref. 16, solid dots) with the result of Eq. (4.2), averaged over the random background charge (open squares with error bars). We used identical gate and junction capacitances, with $C_g/C=0.044$ ($N_c=12$), as estimated in Ref. 16. There are no adjustable parameters.

The crossover to a linear N dependence supports the intuitive idea that the background charge in the array is screened beyond N_c. The rms deviation $\mathrm{rms}V_t = 0.31e(\sqrt{N}-1)/(2C+C_g)$ for all N. The rms deviation of the threshold voltage for tunneling through a specific junction k has a much stronger dependence on N than $\mathrm{rms}V_t$ itself: $\mathrm{rms}V_{t,k} \propto N^{3/2}$. Since V_t is chosen as the maximal threshold voltage in a sequence of N minimal values for single tunneling events, the fluctuations in V_t are smaller than those in $V_{t,k}$. In Fig. 3 we compare the threshold voltage from Eq. (4.2), averaged over all background charges, with experimental threshold voltages for arrays of different lengths.[16] We used the values $C=0.28$ fF and $C_g=0.012$ fF from Ref. 16, giving $N_c=12$. Thus, the experimental results are in the regime of a linear dependence of $\langle V_t \rangle$ on N. The qualitative agreement is satisfactory, without any adjustable parameters.

In conclusion, we have derived an exact analytical expression for the threshold voltage $V_{t,k}(\vec{q})$ for tunneling through a junction k in a one-dimensional array of N metallic islands at arbitrary occupation $\vec{q}$ of the islands. We have calculated the average threshold voltage for transport and its fluctuations in a few simple cases. In particular, we have found that including random background charges results in a N^a dependence of $\langle V_t \rangle$, with $a=\frac{1}{2}$ for $N<2.5\sqrt{C/C_g}$ and $a=1$ for $N>2.5\sqrt{C/C_g}$. We have made a comparison with the available experimental data on gated one-dimensional arrays,[16] and found a reasonable agreement.

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*Present address: Department of Theoretical Physics, Lund University, Sölvegatan 14A, 22362 Lund, Sweden.

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