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

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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\[2] 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] ultradense integrated digital electronics,\[4] thermometry,\[5] and room-temperature memory.\[6] In many of these applications, tunneling occurs through a large number of junctions in series. Most theoretical work has assumed homogeneous arrays.\[2] 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.\[2] 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 non-uniform background charges on the islands. This is relevant, since the charging energy is very sensitive to the background charge.

The aim of this article 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,\[2] 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 Section II the change in the free energy of an $N$-junction array due to an arbitrary tunneling event. In Section 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 $\langle V_t \rangle = \frac{1}{2}Ne(C^{-1})$, with $(C^{-1})$ being typically not much different from $1/\langle C \rangle$. However, as we show in Section 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.\[2]

II. FREE ENERGY

![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 $C_{i,i+1}$, 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.](image-url)
The system under consideration is shown schematically in Fig. 3. Within the orthodox model, the state of the system is described by the numbers $n_i$ of electrons on the $i$-th 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:

$$\Gamma_k(\vec{n}) = \frac{\Delta G_k(\vec{n})}{e^2 R_k[1 - \exp(-\Delta G_k(\vec{n})/k_B T)]}. \quad (1)$$

Here $R_k$ is the resistance of the $k$-th 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:

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

We denote by $\phi_i$ 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:

$$Q_e = C_1(V_e - \phi_1) + e n_e, \quad (3a)$$
$$Q_c = C_N(V_c - \phi_{N-1}) + e n_c, \quad (3b)$$
$$Q_{g,i} = C_{g,i}(V_{g,i} - \phi_i). \quad (3c)$$

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 $Q_{0,i}$:

$$\Delta G_k(\vec{n}) = -\frac{e^2}{2} (R_{k-1,k-1} + R_{k,k} - R_{k-1,k} - R_{k,k-1}) + e \sum_{i=1}^{N-1} Q_i(R_{i,k-1} - R_{i,k})$$
$$+ e(V_e - V_{g,1}) A_{1,k} + e \sum_{i=2}^{N-1} (V_{g,i-1} - V_{g,i}) A_{i,k} + e(V_{c,N-1} - V_c) A_{N,k}, \quad (9a)$$

$$A_{i,k} = C_i(R_{i-1,k} + R_{i,k} - R_{i-1,k-1} - R_{i,k}) + \delta_{i,k}. \quad (9b)$$

Here, $R_{i,N} = R_{0,i} = 0$ is implied.

Although we are now able to construct all relevant transition rates from expressions (1) and (3), 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 \( D' \), following from Eq. (8), have a simple form. For convenience, we introduce the notation

\[
S_k = \sum_{i=k+1}^{l} \frac{1}{C_i}, \quad S' = S_0', \quad S_k \equiv S_k'.
\]

In terms of these quantities,

\[
D_k = C_1C_2 \cdots C_{k+1}S_{k+1}', \quad D'_{k} = C_kC_{k+1} \cdots C_NS_{k-1}', \quad R_{i,j} = S'_{i,j}S'/S'^{N}, i \leq j.
\]

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:

\[
V_{t,k}(\vec{q}) = \frac{e}{2} \left( S'N - \frac{1}{C_k} \right) - e \sum_{i=1}^{k-1} q_i S_i' + e \sum_{i=k}^{N-1} q_i S_i. \tag{12}
\]

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

\[
V_t = \frac{e}{2} \left( \sum_{i=1}^{N} \frac{1}{C_i} - \text{Max}[1/C_1, 1/C_2, \ldots, 1/C_N] \right), \tag{13}
\]

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

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

\[
R_{i,j} = (S_i' + C_g S_n')S_j'(S_i' + C_g S_n')^{-1}, \quad n \leq i \leq j
\]

\[
R_{i,j} = S_i'S_j(S_i' + C_g S_n')^{-1}, \quad i \leq n \leq j
\]

\[
R_{i,j} = S_i'(S_j + C_g S_n')S_i(S_i' + C_g S_n')^{-1}, \quad i \leq j \leq n
\]

\[
R_{i,j} = R_{j,i}.
\]

In order to determine the threshold voltage \( V_{t,k}(\vec{q}) \), we have to distinguish between \( k \leq n \) and \( k > n \). From Eqs. (10) and (11), we find that \( V_{t,k}(\vec{q}) \) now depends on the gate voltage \( V_g \).

\[
V_{t,k}(\vec{q}) = \frac{e}{2} \left( S'N - \frac{1}{C_k} \right) - e \sum_{i=1}^{k-1} q_i S_i' + e \sum_{i=k}^{N-1} q_i S_i' + C_g[V_g - \frac{e}{2}(V_e + V_c)] \times \begin{cases} S_n(1 + \frac{1}{2}C_g S_n)^{-1}, & k \leq n \\ -S_n'(1 + \frac{1}{2}C_g S_n')^{-1}, & k > n \end{cases}
\]

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 \((C_i = C \text{ for all } i)\). We start by investigating an array with a non-zero 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.\(^4\)

In the absence of gate coupling \((C_{g,i} = 0 \text{ for all } i)\) and for a non-zero 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:

- transfer of an electron from the emitter to the first island (electron injection through junction \(k = 1\));
- 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 \(m\));
- 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

\[
V_t = \frac{e}{2C} (N - 1 - 2\min[mq_{0,m}, (N - m)(1 - q_{0,m})]) ,
\]

where

\[
q_{0,m} \geq 0,
\]

or

\[
V_t = \frac{e}{2C} (N - 1 - 2\min|m(1 - |q_{0,m}|), (N - m)|q_{0,m}|) ,
\]

where

\[
q_{0,m} < 0.
\]

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 \((V_t) = (5N - 7)e/12C\), with variance \(\text{Var}(V_t) = (e/2C)^2(3N^2 - 5N + 8)/180N\). 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 \(\text{rms}V_t \propto Ne/C\), of the same order as the threshold voltage itself.

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\[
V_{t,k} = \frac{e}{2C} \left( -2 \sum_{i=1}^{k-1} (q_i + q_g) \sinh(i\lambda) \cosh((N - k + \frac{1}{2})\lambda) + 2 \sum_{i=k}^{N-1} (q_i + q_g) \sinh((N - i)\lambda) \cosh((k - \frac{1}{2})\lambda) \right) \left( \sinh \lambda \cosh \frac{NL}{2} \cosh \frac{(N - 2k + 1)\lambda}{2} \right)^{-1}.
\]

Here, the gate-induced charge \(q_g = C_g[V_g - \frac{1}{2}(V_e + V_c)]\) 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

\[
\langle V_t \rangle = e/(4C + 2C_g).
\]

In the absence of background charges and for \(q_g = 0\), we find

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

which approaches a constant value as \(N \to \infty\), provided \(\lambda \neq 0\), i.e. provided \(C_s/C \neq 0\). In Figure 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. (18). 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 (20) 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 cross-over to
a linear $N$-dependence for large arrays. For $C_g \ll C$, the
array length $N_c$, at which the cross-over occurs is found
to be 2.5 times the soliton width,
\begin{equation}
N_c \approx 2.5 \sqrt{C/C_g} \approx 2.5 \lambda^{-1}.
\end{equation}

For $N < N_c$ the average threshold voltage is well de-
scribed by an extrapolation of the result (19) for $N = 2$:
\begin{equation}
\langle V_t^\leq \rangle = \frac{e}{4C + 2C_g} \sqrt{N - 1}/\sqrt{2 - 1}.
\end{equation}

For $N > N_c$ we can describe the numerical data by
\begin{equation}
\langle V_t^\geq \rangle = \langle V_t^\leq \rangle \bigg|_{N=N_c} + (N - N_c) \frac{d\langle V_t^\leq \rangle}{dN} \bigg|_{N=N_c}.
\end{equation}

The cross-over to a linear $N$-dependence supports the
intuitive idea that the background charge in the array
is screened beyond $N_c$. The rms deviation $\text{rms}V_t = 0.31 e (\sqrt{N} - 1)/(2C + C_g)$ 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 $\text{rms}V_k$ itself: $\text{rms}V_{t,k} \propto N^{3/2}$. 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 $V_{t,k}$.

\begin{align*}
\text{FIG. 3} & \quad \text{Comparison of experimental threshold voltages (taken from Ref. 13, solid dots) with the result of Eq. (18), 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.}
\end{align*}

In Figure 3 we compare the threshold voltage from
Eq. (18), averaged over all background charges, with experimental threshold voltages for arrays of different lengths.\textsuperscript{14} We used the values $C = 0.28 \text{ fF}$ and $C_g=0.012 \text{ fF}$ 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 $V_{t,k}(\bar{q})$ for tunnel-
ing through a junction $k$ in a one-dimensional array of $N$
metallic islands at arbitrary occupation $\bar{q}$ 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 $a = 1/2$ 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\textsuperscript{13} and found a reasonable agreement.

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