Exact Solution of the Electrostatic Problem for a Single Electron Multijunction Trap

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We present an exact solution for the potential profile of a biased single electron trap. Analytical expressions for the total free energy as well as the corresponding charging energy, barrier height for a trapped electron in the store island, and threshold voltage for a single charge transfer are derived. This enables us to demonstrate the important role of well capacitance C_w in determining the barrier height of the trapped electron, and to show that systems with small well capacitance are not suitable for studying the single electron trap. Our techniques are applicable to a variety of other single charge tunneling systems.

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Recent advances in nanotechnology [1,2] have made it possible to fabricate arrays of small tunnel junctions, which exhibit the Coulomb blockade effect. Among the systems being discussed [1], there are the "turnstile," where a gate electrode controlled by an rf signal is capacitively coupled to the center of the array, and the "pump," where two gate electrodes controlled by two rf signals are capacitively coupled to the electrodes inside the array. These two kinds of devices have been used to transfer, with the help of the Coulomb blockade effect, a controlled number of electrons into a capacitor, and are promising as candidates for a charge standard for possible metrological applications and digital devices [1,2]. However, it is known that the Coulomb blockade can never be complete, and thus for possible metrological applications of these two devices, it is crucial to know the error rate of the operation, which depends on how frequent and by what processes the electrons transit the device in the presence of a Coulomb barrier. In order to study the barrier confinement, a special device structurally similar to the turnstile and pump, the single electron "trap," where the end of the array is connected to a well capacitor, has been studied by many authors [3–8]. One of the basic questions in studying the single electron trap is the evaluation of the barrier height for the trapped electron. Whereas numerous papers have been published [2–8] on this subject, there are still some important questions which remain unanswered. For example, the role of the well capacitance C_w (see Fig. 1 and the later discussion) in determining the barrier height is not clear: In Refs. [2,3] the small well capacitance C_w region ($C_w/C < 1$)) has been studied, while in Refs. [4–8] it is in the opposite region. The purpose of this Letter is to focus our attention on the question of how to study the consequent barrier confinement of the single electron trap in a precise way, and to provide some insightful analysis by presenting an exact analytical solution to the electrostatic problem of the single electron trap consisting of a finite but arbitrary number of small gated junctions, with equal junction capacitances C and equal gate capacitances C_g. These analytical results enable us to demonstrate the important role of C_w in determining the barrier height of the trapped electron, and to show that the systems with small well capacitance C_w are not suitable for fabricating a high quality single electron trap.

The system with which we are concerned, the single electron trap, is illustrated in Fig. 1, where the bias voltage of the left edge is $\Phi_0 = V$ and that of the right edge is $\Phi_{N+1} = U$. We denote the potential on each of the individual $N - 1$ islands between the junctions in the array by the column vector $\overline{\Phi} = \{\Phi_1, \Phi_2, \ldots, \Phi_{N-1}\}^T$, and the number of excess electrons on each of the individual $N - 1$ islands is denoted by the column vector $\overline{n} = \{n_1, n_2, \ldots, n_{N-1}\}^T$. In addition, we denote the potential and the number of the excess electrons on the *store island* between the nth junction and the well capacitor as Φ_N and n_N, respectively. The island potentials $\{\overline{\Phi}, \Phi_N\}$ and the number of the excess island electrons $\{\overline{n}, n_N\}$ are related by the charge conservation law and Kirchhoff's law, and they obey a set of N linear equations [9]. These linear equations can be conveniently put into a simple matrix form

$$\begin{pmatrix} \overline{\overline{M}} & \overline{1} \\ \overline{1}^T & D' \end{pmatrix} \begin{pmatrix} \overline{\Phi} \\ \Phi_N \end{pmatrix} = \frac{e}{C} \begin{pmatrix} \overline{n} \\ n'_N \end{pmatrix}, \tag{1}$$

where

$$D' = -1 - (C_w + C_c)/C .$$

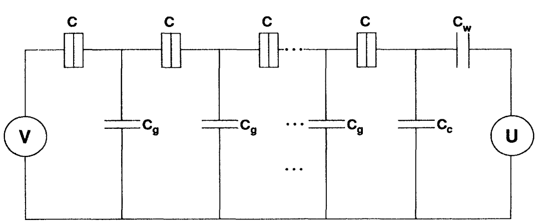

FIG. 1. Schematic of a single electron trap which consists of N small tunnel junctions in series, with equal gate capacitances C_g, and equal junction capacitances C, the end of which couples to a well capacitance C_w, and an input gate capacitance C_c. The bias voltage of the left edge is V and that of the right edge is U.

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Also, in (1) the column vector $\overline{1} = \{0, 0, \ldots, 1\}^T$ has $N - 1$ elements, and the matrix $\overline{\overline{M}}$ is an $N - 1$ by $N - 1$ symmetric tridiagonal matrix, having the same diagonal elements $D = -2 - C_g/C$, and the same off-diagonal elements 1. In addition, the symbol n_N' stands for $n_N - C_w U/e$ and the first element of $\overline{n}$ in (1) is understood to be $n_1 - CV/e$, to accommodate the effects of the bias voltages.

We find that (1) can be solved analytically, and the result is

$$\begin{pmatrix} \overline{\Phi} \\ \Phi_N \end{pmatrix} = -\frac{e}{C} \begin{pmatrix} \overline{\overline{B}} & \frac{-1}{D'+R_{N-1}} \overline{R} \\ \frac{-1}{D'+R_{N-1}} \overline{R}^T & \frac{-1}{D'+R_{N-1}} \end{pmatrix} \begin{pmatrix} \overline{n} \\ n_N' \end{pmatrix}$$
$$= -\frac{e}{C} \overline{\overline{R'}} \begin{pmatrix} \overline{n} \\ n_N' \end{pmatrix}, \qquad (2)$$

where the element of the column vector $\overline{R}$ is given by

$$R_i = \frac{\sinh i\lambda}{\sinh N\lambda}, \qquad (3)$$

with λ defined by

$$-2\cosh\lambda = D = -2 - C_g/C. \qquad (4)$$

In addition, in (2) the element of the N by N symmetric matrix $\overline{\overline{R'}}$ is given by

$$R_{ij}' = B_{ij} = (-1)^{i+j+1} \frac{M_{N-1-j}' M_{i-1}}{M_{N-1}'},$$
$$\text{for } i \leq j, \quad \text{and} \quad i, j \leq N - 1, \qquad (5)$$

with

$$M_{j+1}' = G M_j - M_{j-1}, \qquad (6a)$$

and

$$M_j = (-1)^j \frac{\sinh(j + 1)\lambda}{\sinh\lambda}, \qquad G = D - 1/D'. \qquad (6b)$$

We note that in our notation, $\overline{\overline{B}}$ is an $N - 1$ by $N - 1$ symmetric submatrix to $\overline{\overline{R'}}$. Also we note that the R_i of (3) is the same as the matrix element $R_{i,N-1}$ appearing in the problem of 1D array of N tunneling junctions with equal capacitances and $N - 1$ equal gate capacitances [9]. One can easily check that when $C_c = C_g$ and $C_w = C$, the R_{ij}' of (2) reduces to the corresponding form of a 1D array with $N + 1$ equal capacitances C and N equal gate capacitances C_g as studied in Ref. [9].

Equation (2), supplemented by (3)–(6), is a key result of this paper. By using it one can evaluate the free energy of the 1D trap analytically. Since the free energy is a crucial quantity in determining the rate of tunneling in small junctions, one needs to define it in a precise way. Basically, the free energy contains two terms, the electrostatic energy and the work done in moving the charged soliton through the system. For a biased single electron trap as illustrated by Fig. 1, the Gibbs free energy as a function form of the charge profile $\{\overline{n}, n_N\}$ can be written as

$$F = E_0 + \frac{e^2}{2C} \sum_{i,j=1}^{N} n_j R_{ij}' n_j - VQ_0 - UQ_{N+1}, \qquad (7)$$

where the first two terms in the right-hand side originate from the charging energy, with E_0 a quantity independent of the charge profile $\{\overline{n}, n_N\}$. In addition

$$Q_0 = n_0 e + C(V - \phi_1),$$
$$Q_{N+1} = n_{N+1} e + C_w(U - \phi_N). \qquad (8)$$

Also, the local voltage $V_i = \Phi_{i-1} - \Phi_i$, with $\Phi_0 = V$ and $\Phi_{N+1} = U$.

Equation (7) is a general expression for the Gibbs free energy of a single electron trap with bias voltages $\{V, U\}$, charges $e\{\overline{n}, n_N\}$, and potential profile $\{\overline{\Phi}, \Phi_N\}$ on the islands. First, we study the charging energy $E_c(k)$ of the system when there is an excess electron on the kth island. In this case, one has $n_i = \delta_{ik}$, and the charging energy term in (7) reduces to

$$E_c(k) = E_0 + e^2/2CR_{kk}', \qquad (9)$$

where E_0 is the same as (7), and R_{ij}' is given by (5). In Fig. 2, we plot $E_c(k)$ vs k at three different values of $(C_c + C_w)/C = 0.1$, 1, 10, and $C_g/C = 0.01$, 0.1, 1. As can be seen from the figure, when $C_c + C_w$ is close to $C_g + C$ [see the curve at $(C_c + C_w)/C = 1$ and $C_g/C = 0.01$], one has $E_c(k) = E_c(N + 1 - k)$. In this case, the $E_c(k)$ of the middle island ($k = 4$) has the maximum value, and an electron can be trapped in the store ($k = 7$) island. An increase in the value of $C_c + C_w$ [see the curves at $(C_c + C_w)/C = 10$] will further increase the barrier height of the trapped electron. Thus, when $(C_c + C_w)/C$ is large and C_g/C is small, it is

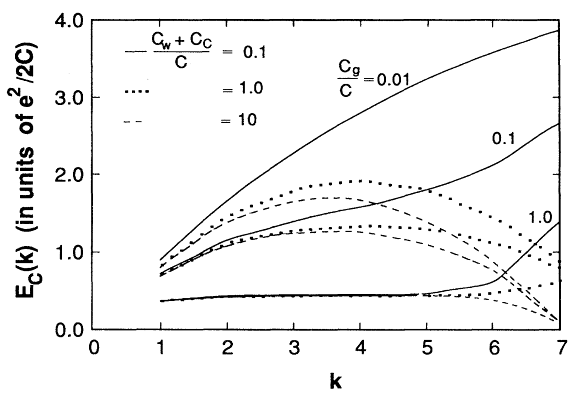

FIG. 2. Charging energy $E_c(k)$ (in units of $e^2/2C$) for a single electron trap with an excess electron at the kth island, as a function of k at three different values of $(C_c + C_w)/C$: 0.1 (full curves), 1 (dotted curves), 10 (dashed curves), and $C_g/C = 0.01$, 0.1, 1 (from top to bottom). Also C, C_g, C_w, and C_c, are the junction capacitance, gate capacitance, well capacitance, and input gate capacitance, respectively. For clarity of illustration, we have treated k as a continuous variable whereas only the integer values are of physical interest.

in favor of trapping electrons in the store island. On the other hand, when $(C_c + C_w)/C$ is small [see the curves at $(C_c + C_w)/C = 0.1$], $E_c(k)$ increases with increasing k, and no electron can be trapped in the store island.

Another interesting feature of (9) is that one can now evaluate analytically the barrier height of the trapped electron. For this purpose, it is easy to show from (9) that the charging energy $E_c(k)$ of (9) takes its maximum value at the position

$$k_m = \frac{1}{2}\left[N - 1 + \frac{1}{2\lambda}\ln\frac{1 + D'e^{\lambda}}{1 + D'e^{-\lambda}}\right], \tag{10}$$

subject to the conditions

$$\frac{C_w + C_c}{C} > \frac{\sinh(N+1)\lambda}{\sinh N\lambda} - 1, \tag{11a}$$

$$C_g < \frac{(C_w + C_c)^2}{C + C_w + C_c}. \tag{11b}$$

In the above evaluation we treated k_m as a continuous variable, whereas it is an integer. Thus, to get the position where the barrier height is a maximum, we should take the closest integer to the value given by (10). We note that (11a) is derived from the fact that the last term in the bracket in (10) should be less than $N + 1$ so that the k_m of (10) can be no greater than N, while (11b) is obtained from the condition that the arguments of the logarithmic function in (10) should be greater than zero. Also, from (10) it is easy to show that in the $C_g = 0$ limit, k_m tends to the value of $\frac{1}{2}[N - 1/(1 + D')]$. Since k_m cannot be larger than N this latter relation indicates that in the $C_g = 0$ limit, in order to trap an electron in the store island, it is necessary to have $N(C_w + C_c) > C$.

The exact value of the barrier height ΔE can be obtained from (9) as [subject to the conditions (11)],

$$\Delta E \equiv \frac{e^2}{2C}(R'_{k_m k_m} - R'_{NN}) = \frac{e^2}{2C}\left(\frac{\tanh k_m\lambda}{2\sinh\lambda} + \frac{\sinh N\lambda}{D'\sinh N\lambda + \sinh(N-1)\lambda}\right). \tag{12}$$

Here k_m is understood to be the closest integer to the value given by (10). In the $C_g = 0$ limit, (12) reduces to a simple form

$$\Delta E = \frac{e^2}{2C}\frac{[N(1 + D') + 1]^2}{4(1 + D')[N(1 + D') - 1]}, \quad \text{for } \frac{C_w + C_c}{C} > \frac{1}{N}, \tag{13}$$

where the listed condition is directly deduced from (11). From (13), it is easy to show that ΔE increases with increasing N or $C_c + C_w$. This is saying that a high barrier for the trapped electron is achieved by increasing either the number of the junctions N or the capacitance $C_c + C_w$. Also, one can now show from (13) that when $C_c = 0$ and $NC_w \gg C$, the barrier height is

$$\Delta E = \frac{e^2}{2C}\frac{N^2 C_w}{4(NC_w + C)}, \quad \text{for } NC_w \gg C. \tag{14}$$

We note that Eq. (14) was previously obtained in Ref. [2] (by using some approximation scheme) without noticing the restrictive condition $NC_w \gg C$. It turns out that in Ref. [3] Eq. (14) has been misused in the region $NC_w < C$, with the particular numbers $N = 7$, $C_w = 10$ aF, and $C = 150$ aF. In fact, with these numbers, one can easily check that the position k_m of the maximum charging energy exceeds the number N, i.e., there cannot be any real trapped electron for that particular system.

The above features of the barrier height ΔE are further illustrated in Fig. 3, where we plot ΔE for two electron traps with $N = 7$ and 10, respectively, as a function of $C_c + C_w$ at three different values of $C_g/C = 0.001$, 0.01, 0.1. As can be seen from the figure, the barrier height ΔE for the trapped electron increases when either the number of the junctions N or the capacitance $C_c + C_w$ increases, or the gate capacitance decreases. Also, the trap conditions as given by (11) are fully illustrated by the figure. In particular, in the small C_g/C limit, the barrier height ΔE disappears, once $(C_c + C_w)/C$ becomes smaller than $1/N$, and it approaches the value of $Ne^2/8C$ in the large $(C_c + C_w)/C$ limit.

Next, we determine the change of the Gibbs free energy ΔF due to some charge transfer event by means of (9). To be definite, here we discuss the case where the charge transfer happened between two islands k and k', while the charges on the other islands are unchanged. We denote the charges on these two islands before and after the charge transfer, respectively, as $\{n_k, n_{k'}\}$ and $\{n'_k, n'_{k'}\}$, and the net transferred charges as Q. After some algebra, we obtain from (11) the change of the Gibbs free energy

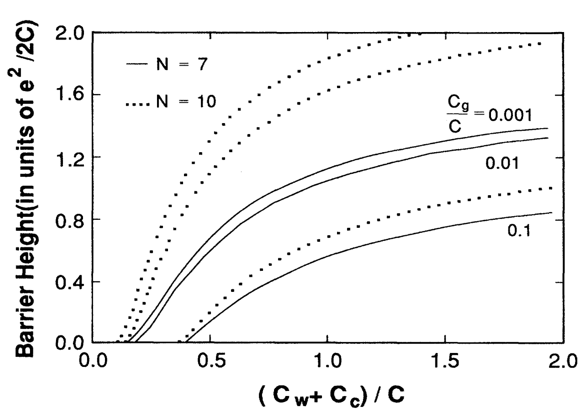

FIG. 3. Barrier height ΔE (in units of $e^2/2C$) of a trapped electron in single electron traps with the number of junctions $N = 7$ and 10, respectively, as a function of $(C_c + C_w)/C$ at three different values of $C_g/C = 0.001$, 0.01, 0.1 (from top to bottom). Also C, C_g, C_w, and C_c, are the junction capacitances, gate capacitances, well capacitance, and input gate capacitance, respectively.

$\Delta F^Q(k,k')$ due to the charge transfer $\{n_k, n_{k'}\}$ to $\{n'_k, n'_{k'}\}$. For the single electron transfer case with $n_i = \delta_{ik}$, $n'_i = \delta_{ik'}$, it reduces to (for convenience, we take $U = 0$)

$$\Delta F^e(k,k') = \frac{e^2}{2C}[R'_{k',k'} - R'_{k,k}] + eV[\delta_{k0} + \delta_{k'0} + R'_{1,k} - R'_{1,k'}], \quad (15)$$

where $R'_{i,j}$ is defined by (5).

The tunneling of a charge soliton from the kth island to the k'th island in the single electron trap is energy favorable when the free energy $\Delta F^e(k,k')$ is less than zero, and vice versa. Thus, the threshold energy V_t for the transfer of a single electron from the kth island onto the k'th island can be obtained by equating $\Delta F^e(k,k') = 0$. Applying this principle to (15), for the single electron transfer case, we obtain

$$V_t(k,k') = -\frac{e}{2C}\frac{R'_{k',k'} - R'_{k,k}}{R'_{1,k} - R'_{1,k'} + \delta_{k0} + \delta_{k'0}}. \quad (16)$$

Equation (16) is an interesting result. By using (16) one immediately finds that in the nearest neighbor tunneling sequence ($k \leftrightarrow k+1$), the absolute value of $V_t(0,1)$ is the largest for an electron tunneling into the trap, while $V_t(N,N-1)$ is the largest for an electron escaping from the trap. This implies that the actual tunneling threshold voltage and the actual escape threshold voltage are, respectively, $V_t(0,1)$ and $V_t(N,N-1)$. In the $C_g \ll C$ limit, by using (3)–(6), we obtain from (16)

$$V_t(0,1) = -\frac{e}{2C}\left(N - 1 + \frac{C}{C_w + C_c}\right), \quad (17)$$

$$V_t(N,N-1) = \frac{e}{2C}\left(N - 1 - \frac{C}{C_w + C_c}\right). \quad (18)$$

Note that there is a sign difference between the tunneling threshold voltage (17), a negative value which enables the tunneling of an electron, and the escape threshold voltage (18), a positive value which helps the escape of an electron. Equations (17) and (18) indicate that in the large $(C_w + C_c)/C$ limit, the magnitude of both threshold voltages tends to the value of $(N-1)e/2C$, which increases linearly with the number of junctions in the system. In other words, in the small C_g/C and large $(C_w + C_c)/C$ limits, electrons can hardly tunnel through or escape from the single electron trap consisting of a large number of junctions. Also, (17) and (18) are subject to the conditions (11), i.e., in the small $C_w + C_c$ limit $[(C_w + C_c)/C < 1/N]$, there will be no trapped electrons, and the threshold voltage V_t loses its meaning.

In summary, in this paper we have presented an exact solution (2) for the potential profiles of a biased single electron trap which consists of N gated small junctions with equal gate capacitances, and equal junction capacitances, the end of which couples to a well capacitance. Our study shows that in the small well capacitance limit $[(C_w + C_c)/C < 1/N]$, the potential profile of a single electron trap does not show a barrier height, and there will be no trapped electrons. Also, we have identified the conditions (11a) and (11b) for the values of gate and well capacitances for which the electron can actually be trapped. In particular, we have shown that the well known formula (14) for the barrier height is true only in the region where the condition $NC_w \gg C$ is satisfied. Finally, we note that our techniques are applicable to a variety of other single charge tunneling systems.

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