Hysteretic voltage gap of a multijunction trap

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The hysteretic voltage gap $\Delta V^{(m)}$, the difference between the threshold voltages for electrons to tunnel into and escape from a single-electron trap (which consists of N gated small junctions with equal junction capacitances C, equal stray capacitances C_0, and well capacitance C_w) through an m-junction cotunneling process, is studied. By using an exact solution of the potential profiles [Phys. Rev. Lett. **74**, 1839 (1995)], we find that $\Delta V^{(m)}$ has a strong dependence on m, C_0/C, C_w/C, and N, and that the hysteresis loop does not exist beyond a critical value β of C_0/C. Previous discussions in the literature have neglected the effect of the stray capacitances but we find that even comparatively small values have a large effect (especially for small C_w and large N) and, in particular, their inclusion was necessary to explain the ΔV obtained in some recent experiments [Phys. Rev. Lett. **72**, 3226 (1994)]. [S0163-1829(96)03128-1]

The Coulomb blockade[1,2] of tunneling in small tunnel junctions has led to the design and operation of devices in which electrons are transported in a controlled fashion. One of the most significant systems being studied by many authors[3–12] is the single-electron ''trap'' (see Fig. 1 in Ref. 11). Whereas numerous papers have been published on this subject, there are still some important questions which remain unanswered. For example, the role of the well capacitance C_w in determining the barrier height is not clear: in Refs. 2–4 the small C_w region ($C_w/C<1$, where C is the junction capacitance) has been studied, while in Refs. 5–9 it is in the opposite region. In addition, the effect of the stray capacitance C_0, which is known to be important in determining the soliton width in a one-dimensional array, has not been fully explored. The purpose of this paper is to present 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 C and equal C_0. We are especially interested in explaining the hysteretic voltage gap in Fig. 2 of Ref. 3.

Our starting point here is the Gibbs free energy of a biased single-electron trap, which can be written as[11]

$$F=E_0+\frac{e^2}{2C}\sum_{i,j=1}^{N} n_i R'_{ij} n_j - VQ_0 - UQ_{N+1}, \tag{1}$$

where V is the bias voltage, U is the gate voltage on the well capacitance, n_i is the number of excess electrons on the ith island, and R'_{ij} is a matrix element which depends on C, C_0, and C_w. For detailed expressions for R'_{ij}, E_0, Q_0, and Q_{N+1}, we refer to Eqs. (5)–(8) in Ref. 11.

Equation (1) is a general expression for the F of a single-electron trap with bias voltages $\{V,U\}$, and charges $e\{\overline{n,n_N}\}$ on the islands. Based on (1), one can study in detail the change of the Gibbs free energy ΔF due to some charge-transfer event. As we mentioned earlier, there are N islands which we label $k=1,2,\ldots,N$. We now also use $k=0$ to denote the left edge. In this context, we define

$$R'_{oi}=R'_{io}=0, \tag{2}$$

and use (1) to calculate ΔF due to some charge-transfer event from the left edge to the islands as well as between the islands in the trap.

We now study the $T=0$ *threshold voltage* V_t for the transfer of a single electron from the k island onto the k' island, which is obtained by equating $\Delta F=0$. From (1) we obtain (for convenience, we take $U=0$)

$$V_t(k,k')=-\frac{e}{2C}\frac{R'_{k',k'}-R'_{k,k}}{R'_{1,k}-R'_{1,k'}+\delta_{k0}+\delta_{k'0}}. \tag{3}$$

By using (3) one immediately finds that in the m-junction tunneling sequence ($k\leftrightarrow k+m$), the absolute value of $V_t(0,m)$ is the largest for an electron tunneling into the trap, while $V_t(N,N-m)$ is the largest for an electron escaping from the trap. This implies that for the m-junction tunneling events, the tunneling threshold voltage and the escape thresh-

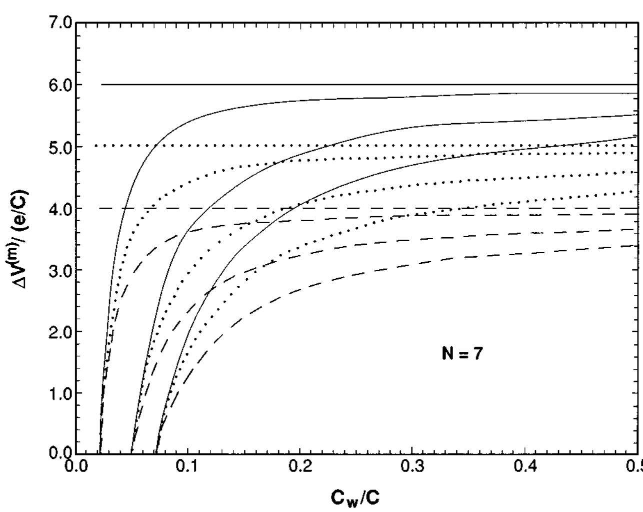

FIG. 1. The hysteretic voltage gap $\Delta V^{(m)}$ (in units of e/C) for the mth-order cotunneling process in a single-electron trap which consists of $N=7$ small tunnel junctions, as a function of C_w/C as calculated from (6) at $C_0/C=0$, 0.001, 0.005, 0.01 (from top to bottom) and $m=1$ (full lines), 2 (dotted lines), 3 (dashed lines). Here C, C_0, and C_w are the junction capacitances, stray capacitances, and well capacitance, respectively.

old voltage at $T=0$ are, respectively, $V_t(0,m)$ and $V_t(N,N-m)$, which, using (3), can be written as

$$V_t^{(m)}(0)\equiv V_t(0,m)=-\frac{e}{2C}\frac{R'_{mm}}{1-R'_{1m}}, \quad (4)$$

$$V_t^{(m)}(N)\equiv V_t(N,N-m)=-\frac{e}{2C}\frac{R'_{N-m,N-m}-R'_{N,N}}{R'_{1,N}-R'_{1,N-m}}. \quad (5)$$

Equations (4) and (5) are general forms for the m-junction cotunneling process,[7] where electrons tunnel across m junctions at the same time. When $m=1$, it becomes the special case of one-junction tunneling. Also, from (4) and (5) it can be shown that in general the higher-order cotunneling process has a lower V_t than that of the lower-order process. For example, in the $C_0\rightarrow 0$ limit, one can easily show that (4) reduces to $V_t^{(m)}(0)=-(e/2C)(N-m+1/x)$, where $x=(C_w+C)$. In this case, if one takes $N=7$ and $x=\frac{1}{15}$, then $V_t/(-e/2C)=21$ for single-junction tunneling while $V_t/(-e/2C)=19$ for three-junction tunneling. In other words, when the single-junction tunneling is completely blocked at certain bias voltages, some higher-order multijunction cotunneling processes are still possible even though the corresponding rate of tunneling is considerably lower.[7]

An interesting phenomenon of the multijunction trap as seen in the measured I-V curves[3–6] is the hysteretic loop, i.e., the tunneling and escape of an electron do not occur at the same value of V. Since we have obtained analytic expressions of the threshold voltages for both the tunneling and escape of an electron in the multijunction trap, we can now study the hysteretic phenomenon in a quantitative way and compare the theory directly with experimental results. For this purpose, we introduce the hysteretic voltage gap ΔV, which is defined as the difference between the threshold voltages for the tunneling and escape of an electron in the multijunction trap. By this definition and using (4) and (5), one obtains

$$\Delta V^{(m)}\equiv V_t(N,N-m)-V_t(0,m)$$
$$=-\frac{e}{2C}\left(\frac{R'_{N-m,N-m}-R'_{N,N}}{R'_{1,N}-R'_{1,N-m}}-\frac{R'_{mm}}{1-R'_{1m}}\right), \quad (6)$$

where m denotes the number of junctions the electrons tunnel across. The $\Delta V^{(m)}$ of (6) is a measure of the hysteretic effect of the single-electron trap. When $\Delta V^{(m)}>0$, there is a difference between the threshold voltages for the tunneling and escape of an electron. After tunneling into the system at a voltage above $V_t(0,m)$, the electron cannot escape until the voltage is reduced to $V_t(N,N-m)$. Things are different at $\Delta V^{(m)}<0$, where a reduction of the voltage from $V_t(0,m)$ will immediately result in the escape of the electron, i.e., the electron cannot be trapped in the system. Thus it is important to study the physical behavior of (6), particularly the point at which $\Delta V^{(m)}=0$. In the following, we first study the m dependence of $\Delta V^{(m)}$ and then perform an analysis of the C_0, C_w, and N dependence of $\Delta V^{(m)}$ by taking $m=1$ as example.

The m dependence of $\Delta V^{(m)}$ is illustrated by Fig. 1, where we plot $\Delta V^{(m)}$ of (6) as a function of C_w/C at $N=7$ and $C_0/C=0$, 0.001, 0.005, 0.01 for $m=1$, 2, 3. As can be seen from the figure, as a general rule, the $\Delta V^{(m)}$ at fixed values of C_w/C and C_0/C becomes smaller for larger m. In particular, in the $C_0/C\rightarrow 0$ limit $\Delta V^{(m)}/(e/C)$ tends to the value of $N-m$. Also, at any value of m, $\Delta V^{(m)}$ always decreases with increasing C_0/C, which we now discuss in detail.

First, we perform an analytic analysis for the C_0, C_w, and N dependence of $\Delta V^{(m)}$ by taking $m=1$ as example. For this purpose, it is convenient to rewrite (6) explicitly (we use $\Delta V\equiv\Delta V^{(1)}$ for convenience) as

$$\frac{\Delta V}{e/2C}=\frac{(1+x)\sinh(N-1)\lambda-\sinh N\lambda}{x\sinh\lambda}+\frac{(1+x)\sinh(N-1)\lambda-\sinh(N-2)\lambda}{x[\sinh N\lambda-\sinh(N-1)\lambda]+2(\cosh\lambda-1)\sinh(N-1)\lambda}, \quad (7)$$

where $x=(C_w+C_c)/C$ and $2\cosh\lambda=C_0/C+2$. We note that the parameters contained in (7) are the number of junctions N, the well capacitance C_w, the input capacitance C_c, and the stray capacitance C_0. Since C_w and C_c appear only as additive quantities, one has to study only one of them.

Next, we study the C_0 dependence of ΔV. In the $C_0\ll C$ limit, one can expand (7) with respect of λ, and obtain explicitly

$$\frac{\Delta V}{e/C}=N-1-\lambda^2\left\{\frac{N(N^2-1)}{12}+\frac{N(3N-4)}{4x}+\frac{N-1}{2x^2}\right\}. \quad (8)$$

Equation (8) is an interesting result. First, when $C_0=0$ (corresponding to $\lambda=0$), one obtains the exact value of $\Delta V=(N-1)e/C$, which is known previously for the $N=2$ trap.[1] Secondly, one finds from (8) that ΔV has a strong x dependence: in the small x limit ΔV decreases as a function of x^{-2}. This implies that in estimating ΔV one cannot always neglect the λ^2 term when λ is small ($C_0/C\ll 1$) because the coefficient of this term can be large for either (a) small x (and the smaller C_w the smaller is x) and (b) large number of junctions N. We will return to this particular point below.

We have evaluated (7) at various values of C_0, C_w, and N. In Fig. 2, we plot ΔV as a function of C_0/C at $N=7$ and two different sets of values of C_w/C at (a) 0.05, 0.067, 0.1, 0.5 and (b) 0.5, 1.0, 1.5, 2.0. As can be seen from the figure, when $C_w/C<1$ [see Fig. 2(a)] ΔV takes the maximum value of $(N-1)e/C$ at $C_0=0$, and it decreases with increase of C_0/C. On the other hand, when $C_w/C>1$ [see Fig. 2(b)] ΔV has a more complicated dependence on C_0/C: it reaches its maximum value at some finite C_0/C and then decreases with increase of C_0/C. In general, we have $\Delta V=0$ at a critical value β of C_0/C (for example, β=0.008 at $C_w/C=0.067$ and $N=7$), and the hysteresis loop does not exist once C_0/C is above this critical value β. Also, β takes smaller value when C_w/C becomes smaller. This is to say that for a mul-

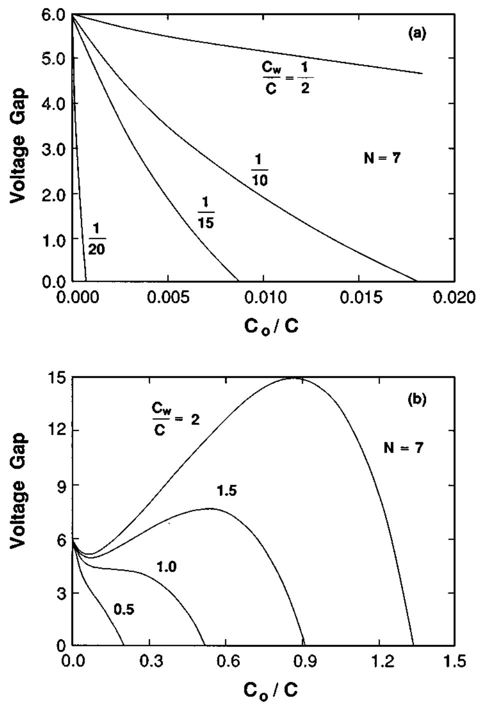

FIG. 2. The hysteretic voltage gap ΔV (in units of e/C) for the single-junction tunneling in a single-electron trap which consists of $N=7$ small tunnel junctions, as a function of C_0/C as calculated from (7) at (a) $C_w/C=0.05$, 0.067, 0.1, 0.5 and (b) $C_w/C=0.5$, 1.0, 1.5, 2.0.

tijunction system with small C_0/C, a small value of C_w/C can significantly reduce or even wipe out the width of the hysteresis loop (for example, $\Delta V=0$ at β=0.008, $C_w/C=0.067$ and $N=7$). Thus β is an important quantity in the consideration of the ΔV of a single-electron trap.

Next, we study the x dependence of β in more detail. By definition, a relationship between x and β can be obtained by using (7) and the condition $\Delta V=0$. After some algebra, we obtain

$$x=[\sqrt{b^2+4ac}-b]/2a, \tag{9}$$

where

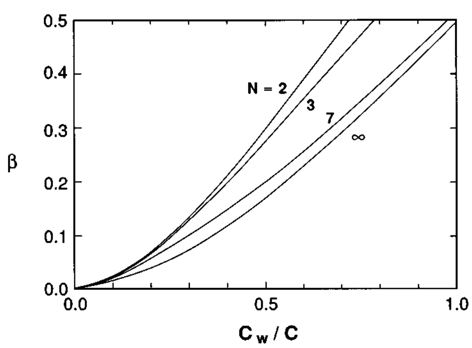

FIG. 3. The critical value β of C_0/C for $\Delta V=0$ as calculated from (9), as a function of C_w/C. For every point above each line there is no hysteresis.

$$a=\sinh(N-1)\lambda[\sinh\lambda+\sinh N\lambda-\sinh(N-1)\lambda], \tag{10a}$$

$$\begin{aligned} b=&2(\cosh\lambda-1)\sinh^2(N-1)\lambda\\ &-[\sinh N\lambda-\sinh(N-1)\lambda]^2\\ &+\sinh\lambda[\sinh(N-1)\lambda-\sinh(N-2)\lambda], \end{aligned}\tag{10b}$$

$$c=2(\cosh\lambda-1)\sinh(N-1)\lambda[\sinh N\lambda-\sinh(N-1)\lambda], \tag{10c}$$

and the relation between β and the corresponding critical value of λ is β=2(cosh $\lambda-1$). In two important limits, (9) reduces, respectively, to the following simple form:

$$\beta=\begin{cases}\dfrac{1}{2}\left\{\dfrac{x^2}{1+x}-1+\left[\left(3+\dfrac{x^2}{1+x}\right)^2-8\right]^{1/2}\right\} & \text{for } N=2 \quad (11)\\[2ex] \dfrac{x^2}{1+x} \quad \text{for } N\lambda\gg 1. & (12)\end{cases}$$

From (11) and (12), it is clear that in general β increases with increasing x. Also, in the $x\to 0$ limit, from (11) one finds that β tends to $2x^2$. It turns out this latter result is valid for any value of N, which can be shown directly from (9). This implies that for a single-electron trap with a fixed stray capacitance $C_0/C\ll 1$, there is no hysteresis voltage gap when the well capacitance C_w/C is smaller than $(C_0/2C)^{1/2}$. Furthermore, in the $x\to\infty$ limit, β tends to $x+1$ (for $N=2$) and x (for $N\lambda\gg 1$), respectively. These features can clearly be seen in Fig. 3, where we plot (9) for β as a function of x for $N=2$, 3, 7, ∞.

The general relationship between β and N is further illustrated in Fig. 4, where we plot β as a function of N calculated from (9) at two different sets of values of C_w/C at (a) 0.05, 0.067, 0.1; and (b) 0.5, 1.0, 1.5. We see that β reaches its minimum value for values of N in the region 5–10 (the larger values corresponding to smaller values of C_w/C), and remains at this value all the way to $N\to\infty$.

In summary, we have presented analytical expressions for the Gibbs free energy (1) and the $T=0$ single charge-transfer threshold voltage (3), for a biased single-electron trap which consists of N gated small junctions with equal stray capacitances and equal junction capacitances, the end of which couples to a well capacitance. The formalism is applied to derive the general expression (6) for the hysteretic voltage gap $\Delta V^{(m)}$ of the mth-order cotunneling process, and to study the m, C_0, C_w, and N dependence of $\Delta V^{(m)}$. We find that in general the higher-order cotunneling process and the presence of stray capacitances dramatically reduces the hysteretic voltage gap of the single-electron trap. For the single-junction ($m=1$) tunneling process, we have obtained the analytic expression (7) for the hysteretic voltage gap ΔV, and analyzed the C_0, C_w, and N dependence. We find that when $C_w/C<1$, ΔV takes the maximum value of $(N-1)e/C$ at $C_0=0$, and it decreases with increase of C_0/C. For $C_w/C>1$, ΔV reaches its maximum value at some finite C_0/C and then decreases with further increase of C_0/C. In general, at a critical value of $C_0/C=\beta$, we obtain $\Delta V=0$ and the hysteresis loop does not exist beyond this critical value β, which implies that for a multijunction system with

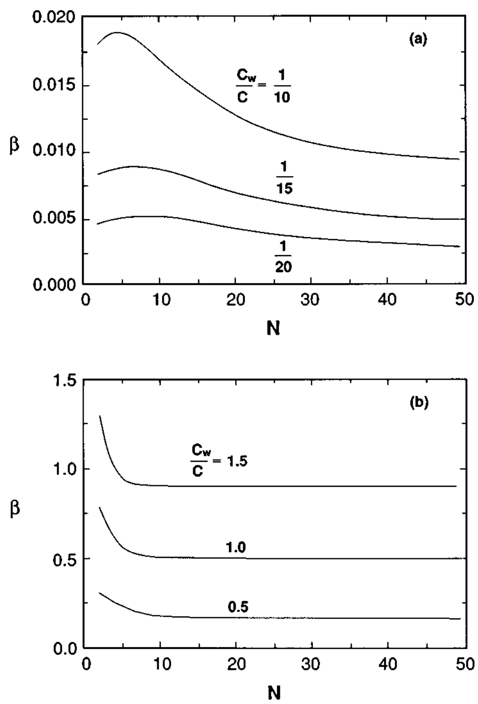

FIG. 4. The critical value β of C_0/C for $\Delta V=0$ as calculated from (9), as a function of N at (a) $C_w/C=0.05$, 0.067, 0.1; and (b) $C_w/C=0.5$, 1.0, 1.5. For every point above each line there is no hysteresis.

small C_w/C, a small value of C_0/C can significantly reduce or even wipe out the width of the hysteresis loop. The $T=0$ theory presented in this paper not only provides a useful starting point in developing a systematic and rigorous theoretical framework for the single-electron trap at finite temperatures, but we find that it also can be used for comparison with existing experimental results, as we will now illustrate.

In the literature, there are many experimental results[3–6] relating to the single-electron trap. These experiments show that well-defined hysteretic voltage gaps ΔV in the I-V curves appear below certain temperatures. Also, the magnitude of the ΔV is system dependent. Since these experiments have different setups, here we compare our theoretical results only to the experimental results of Ref. 3, where no gate control to the islands between the junctions is applied. The values of relevant parameters are[3] $N=7$, $C_w=10$ aF, and $C=150$ aF, and no estimate is given to the value of C_0. The ΔV estimated from the four I-V curves (corresponding to temperatures $T=0.36$, 0.3, 0.21, 0.13 K) appearing in Fig. 2 of Ref. 3 are 0.1, 0.5, 1.0, 1.3 mV, respectively. From these values, one can extrapolate to obtain a $T=0$ value of $\Delta V \sim 1.4$–1.6 mV, which gives an estimate of $\Delta V/(e/C) \sim 1.3$–1.5. This latter number is far less than 6 [the number one would obtain from (10) for single-junction tunneling of an $N=7$ trap with $C_0=0$]. On the other hand, our theoretical results, as presented in Figs. 1 and 2, demonstrate that the presence of the higher-order cotunneling process and the stray capacitance C_0 dramatically reduces the value of ΔV. To determine which order of the cotunneling is effective, one needs to consider both the precision of the relevant experiments and the rate of the cotunneling. In the existing trap experiments[3–6] an electron transition is observable when its rate is greater than of order 1/s to 10^{-2}/s. Also, from the work of Jensen and Martinis[7] it is shown that the cotunneling rates for the $m \geqslant 4$ processes are well below 10^{-2}/s (see Fig. 6 in Ref. 7). Thus it is reasonable to assume that the three-junction tunneling process is responsible for the hysteretic voltage gaps being detected. Now, from Fig. 1 one can readily ascertain the effects, either separately or together, of both stray capacitance and cotunneling, for the system used in Ref. 3. Thus for (a) $C_0=0$ (neglect of stray capacitance) and $m=1$ only (neglect of cotunneling), $\Delta V/(e/C) \sim 6$; (b) $C_0=0$ and $m=3$, $\Delta V/(e/C) \sim 4$; (c) $C_0/C=0.005$ and $m=1$, that $\Delta V/(e/C) \sim 2.5$; (d) $C_0/C=0.005$ and $m=3$, i.e., inclusion of both stray capacitance and cotunneling effects, $\Delta V/(e/C) \sim 1.4$. This clearly demonstrates that the low value of ΔV observed in the experiments of Ref. 3 is a combined effect of the cotunneling and stray capacitance. In fact, neglect of cotunneling would lead to an overestimation of the hysteresis region for this system by about $2e/C$ when $C_0=0$ and $1.1e/C$ when $C_0/C=0.005$.

Finally, we note that in Ref. 12, another scenario of charge transfer is proposed, where the tunneling of a hole into an occupied trap leads to the destruction of the charge state even before the electron barrier is suppressed. However, this is unlikely to account for the big discrepancy between the values of ΔV obtained in the experiments of Ref. 3 and by the simple theory with $C_0=0$ and single-junction tunneling. This is because for hole tunneling to occur it is necessary to have the bias voltage reversed (see Fig. 9 in Ref. 12). Apparently, this is not the case in the experiments of Ref. 12, where the sign of the bias voltage is unchanged (see Fig. 2 in Ref. 3) when one observes the hysteretic voltage gap. In conclusion, in order to understand the ΔV of a single-electron trap, one must consider the effects of both the cotunneling and the stray capacitance.

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