Scaling of the single-electron tunnelling current through ultrasmall tunnel junctions

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Abstract.   The effect of a tunnelling electron on the tunnel barrier shape is studied at the limit where a static image charge model is applicable. It is shown that the single-electron tunnelling current through an ultrasmall voltage-biased junction is not proportional to the junction area because of charging at the electrodes. Simple expressions are presented for the effective static barrier shape of a voltage-biased junction and of a junction in a circuit, the former of which accounts for the anomalous current scaling. A possible experimental arrangement for verifying the scaling relationship is suggested, with numerical results.

A tunnelling electron can affect the tunnel barrier shape, giving rise to such effects as barrier lowering due to the image potential [1]. This effect is independent of the size of the tunnel junction and lowers the barrier energy. In this article, we address the junction-size-dependent influence of a tunnelling electron on the barrier shape. It is caused by electrode charging due to the escape of a single electron into the insulating layer and, as such, becomes appreciable as the size of the electrode is reduced. There has been some controversy over the proper theoretical description of a size-dependent barrier renormalization [2–5], so the issue needs to be subjected to scrutiny. Here we use a simple model that is sufficient to give a clear physical picture of the effect and estimate possible parameters for experimental verification.

We assume that the systems considered have ideal zero-impedance leads and follow the global rule [6] of single-electron transport. The global rule is characterized by the charge redistribution in the entire circuit being so fast that it reaches an equilibrium as soon as tunnelling finishes. We take up two limiting cases: a voltage-biased single junction (figure 1(a)) and a single-electron box [7], which consists of a tunnel junction, a capacitor and a voltage source (figure 1(b)). The single-electron box can be transformed into an equivalent single-junction system with an open switch (SW), shown in figure 2. The voltage source V is provided to give the initial voltage V_i ($=V$) and the switch is kept open throughout the tunnelling event. In general, a tunnel junction in a circuit with one or more isolated islands can be transformed into the equivalent system shown in figure 2. The effective capacitance is given by $C = e/(V_i - V_f)$¶, where V_i is the voltage across the junction before tunnelling begins and V_f is that after tunnelling. For instance, $C = C_j + C_g$ for the single-electron box. The change

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¶ Applicable only if $V_i \neq V_f$—that is, SW is open. C for a voltage-biased junction is the junction capacitance itself.
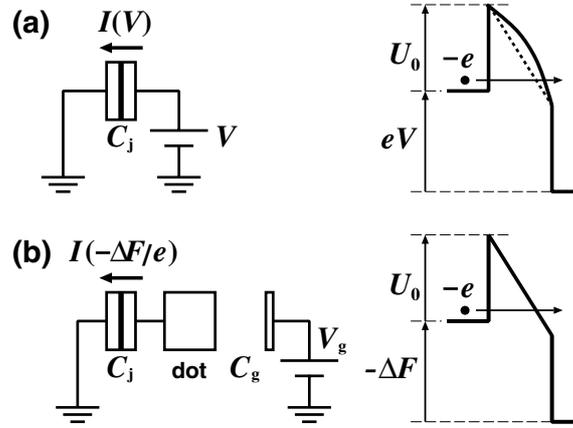
Figure 1. Schematic diagrams of the circuits and the corresponding tunnel barrier profiles considered. The contribution from the image potential is not shown, for clarity. (a) A voltage-biased single junction. The dotted line represents the barrier shape when the charging effect is neglected. (b) A single-electron box.
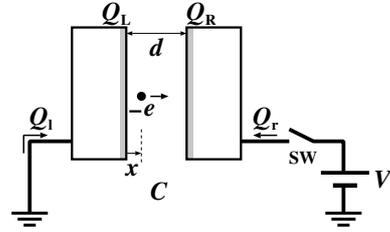

Figure 2. Tunnelling in a parallel-plate tunnel junction.

in electrostatic free energy associated with tunnelling is given by $\Delta F = -\frac{1}{2}e(V_i + V_f)$ whether or not SW is open. If SW is open ($V_i \neq V_f$), we may rewrite this as $\Delta F = -e(CV_i - e/2)/C$, where $e/2$ is the critical charge Q_c [8] for the reduced junction. This expression is related to the better-known expression $\Delta F = -e(Q - Q_c)/C_j$ [8] with $Q = C_j V_i$ and $Q_c = eC_j/2C$.

Now let us look at the barrier shape using the ideal parallel-plate tunnel junction model. Assuming that there is at most one electron within the barrier, we start from the following Hamiltonian:

$$H = \frac{p^2}{2m} + U_b(x) - e\phi_{im}(x) - e\phi_c(x) \tag{1}$$

where $U_b(x)$ is the bare-barrier potential energy, $\phi_{im}(x)$ the normal image potential and $\phi_c(x)$ the scalar potential at x created by electrode charging when the electron is at x. If the barrier traversal time τ_{BL} [9] and the characteristic frequency ω_s of the electrodes' surface excitation modes (e.g. surface plasmons) that couple to the tunnelling electron satisfy the relationship $\omega_s \tau_{BL} \gg 1$, $\phi_{im}(x)$ can be understood in terms of static image charges [1, 10]. Henceforth we assume this condition to be fulfilled.

The difference between $\phi_{im}(x)$ and $\phi_c(x)$ is this. The image potential $\phi_{im}(x)$ actually arises from nonuniform charge distribution on electrode surfaces. The image plane lies in between a charge and its image, so the image charge does not affect the total amount of charge in an electrode nor its voltage. In other words, $\phi_{im}(x)$ originates from the components of the interaction between the electrode charge and the tunnelling charge parallel to the electrode

surfaces. This means that the contribution from the component perpendicular to the electrode surfaces is not included in $\phi_{\text{im}}(x)$. $\phi_{\text{c}}(x)$ is the potential that stems from the perpendicular component. As will be shown below, $\phi_{\text{c}}(x)$ may be size dependent. It is negligible as long as the electrodes are not too small, but could effect a noticeable change in junction characteristics otherwise.

First we examine the voltage-biased single junction (SW closed). The total image charge on the left side of the junction is $Q_{\text{l}} = [1 - (x/d)]e$ and that on the right side is $Q_{\text{r}} = (x/d)e$. Q_{l} and Q_{r} are supplied from the voltage source. These can be derived simply by replacing the electron with a charged conductive plate with the same area as the junction electrodes. $\phi_{\text{c}}(x)$ for closed SW, which we write as $\phi_{\text{c}}^{\text{closed}}(x)$, is given by

$$\phi_{\text{c}}^{\text{closed}}(x) = -\int_0^x (E_{\text{L}} + E_{\text{R}}) \, dx' = -\frac{e}{2C}\left(\frac{x}{d} - \frac{x^2}{d^2}\right) + \frac{Q_0}{C}\frac{x}{d} \tag{2}$$

where $E_{\text{L}} = Q_{\text{L}}/2Cd$, $E_{\text{R}} = -Q_{\text{R}}/2Cd$, $Q_{\text{L}} = -Q_0 + Q_{\text{l}}$, $Q_{\text{R}} = Q_0 + Q_{\text{r}}$ and $Q_0 = CV$.

$\phi_{\text{c}}(x)$ for the single-electron box, which we will write as $\phi_{\text{c}}^{\text{open}}(x)$, can be derived similarly. The only difference is that image charges are not supplied by the voltage source; hence $Q_{\text{L}} = -Q_0 + e$ and $Q_{\text{R}} = Q_0$:

$$\phi_{\text{c}}^{\text{open}}(x) = -\left(\frac{e}{2C} - \frac{Q_0}{C}\right)\frac{x}{d}. \tag{3}$$

In either case, the last term in equation (1) can be identified with the electrostatic free-energy difference ΔF, which is x-dependent in this study. Thus we obtain the following simple prescription for the effective static barrier shape:

$$U_{\text{eff}}(x) = U(x) + \Delta F(x) \tag{4}$$

where $U(x) = U_{\text{b}}(x) - e\phi_{\text{im}}(x)$ and $\Delta F(x) = -e\phi_{\text{c}}(x)$. In the former case (SW closed), Coulomb blockade does not occur because always $\Delta F(d) < 0$ for $V > 0$. In the latter case (SW open), $\Delta F(d) > 0$ if $V_{\text{i}} < e/2C$, and Coulomb blockade does occur. Equation (4) is, therefore, consistent with the generally accepted theory of single-electron tunnelling [11]. It is important to notice that, in the latter, $U_{\text{eff}}(x)$ is different from both the initial and the final barrier shapes. This is crucial for physical validity of the junction's characteristics. Use of either the initial or the final barrier shape can give rise to an unphysical effect, e.g. Maxwell's demon [12].

On comparison of the barrier shapes of the two types of junction under the same effective bias voltage $V_{\text{eff}} = -\Delta F/e$, we find

$$U_{\text{eff}}^{\text{closed}}(x) = U_{\text{eff}}^{\text{open}}(x) + \left(\frac{x}{d} - \frac{x^2}{d^2}\right)\frac{e^2}{2C}. \tag{5}$$

Here $U_{\text{eff}}^{\text{closed}}(x)$ and $U_{\text{eff}}^{\text{open}}(x)$ are the effective static barrier energy $U_{\text{eff}}(x)$ for the 'closed' and 'open' junctions, respectively. Note that V_{eff} is the output of the voltage source that biases the junction if it is voltage biased. In other words, $-\Delta F = eV_{\text{eff}}$ can be regarded as the chemical potential difference across the junction, irrespective of the state of SW (see figure 1). Therefore, if the I–V curve of a voltage-biased junction is given by $I(V)$, that for the same junction in a circuit is $I(V_{\text{eff}})$ [6], supposing the correction which we are dealing with can be ignored.

Equation (3) may be rewritten in a C-independent form as $\phi_{\text{c}}^{\text{open}}(x) = xV_{\text{eff}}/d$, and so be $U_{\text{eff}}^{\text{open}}(x)$ because of equation (4). Consequently, in an 'open' junction, the electron tunnelling rate per unit area from the initial charge configuration, γ_{open}^+, and the rate for the reverse process, γ_{open}^-, do not depend on C for a given V_{eff}†. The current density, defined by $j = e(\gamma^+ - \gamma^-)$‡,

† V_{i} and V_{f} depend on C through $V_{\text{i,f}} = V_{\text{eff}} \pm e/2C$.
‡ j does not describe the dynamical current change within a tunnelling process.

is also independent of C as expected. In contrast, the rates for a 'closed' junction, $\gamma_{\text{closed}}^{+}$ and $\gamma_{\text{closed}}^{-}$, do depend on C as is clear from equation (5). The corollary is that the current density j_{closed} is C-dependent and that the current I_{closed} is not scaled in proportion to the area of the tunnel junction.

Hereafter we concentrate on the 'closed' junction and its current scaling behaviour. Our concern is whether there is a possibility that one can observe it experimentally. It might be observable if $U_{\text{eff}}^{\text{open}}(x)$ and $e^2/2C$ are of comparable order. GaAs/Al$_y$Ga$_{1-y}$As/GaAs tunnel junctions are the systems of choice for the present purpose because it is possible to fabricate very low and thick tunnel barriers that satisfy $\omega_s\tau_{\text{BL}} \gg 1$. This can be done in a well-controlled manner with the use of molecular beam epitaxy [10]. We consider a possible experiment using the following set of parameters: Al content $y = 0.11$, conduction electron concentration in the electrodes $N_D = 10^{18}$ cm^{-3}, barrier thickness $d = 40$ nm and temperature 4.2 K. These will give a conduction band discontinuity of 92 meV, $\omega_s \simeq 4.7 \times 10^{13}$ rad s^{-1}, $\tau_{\text{BL}} \sim 2 \times 10^{-13}$ s and measurable tunnel current at a small bias voltage. We have calculated tunnel current densities by solving a one-dimensional Schrödinger equation using a bulk model. We used an approximate formula for the static image potential proposed by Simmons [13, 14], with a slight modification:

$$\phi_{\text{im}}(x) = \frac{5.75d}{\epsilon_\infty[(m-1)d+x](md-x)} \tag{6}$$

where $\epsilon_\infty \simeq 10.6$ is the high-frequency relative dielectric constant of the barrier layer and m is a constant slightly larger than unity†. In equation (6), d and x are in ångströms and $\phi_{\text{im}}(x)$ is in volts. Shown in figure 3 is the normalized closed-current density $K = j_{\text{closed}}/j_{\text{open}}$ as a function of the effective capacitance C. Were it not for the last term in equation (5), K would be unity. This result suggests that the effect could be noticeable at $C \sim 10^{-16}$ F or less. One could check the scaling behaviour by preparing two voltage-biased tunnel junctions with different areas and comparing the currents that flow through them. Figure 4 shows the tunnel currents and K with respect to the net junction area A, which excludes the depletion

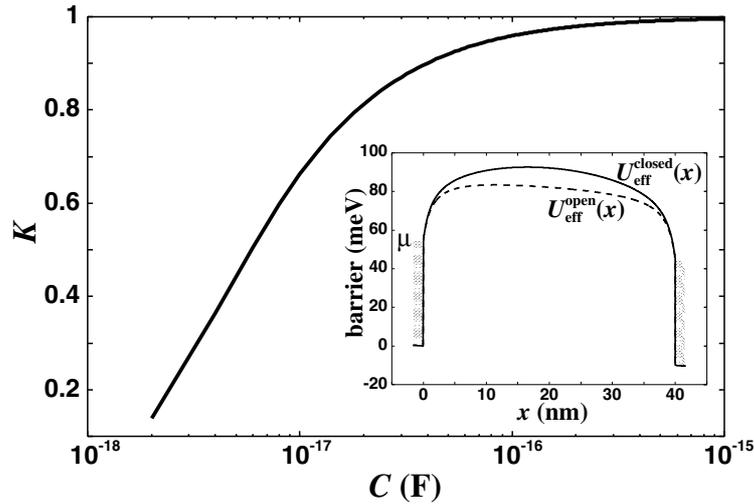† Strictly, d is the distance between the image planes.

Figure 3. $K = j_{\text{closed}}/j_{\text{open}}$ versus $C = \epsilon_\infty\epsilon_0 A/d$ with constant d. The inset shows the corresponding barrier shapes at $C = 2$ aF. $V_{\text{eff}} = 10$ mV.
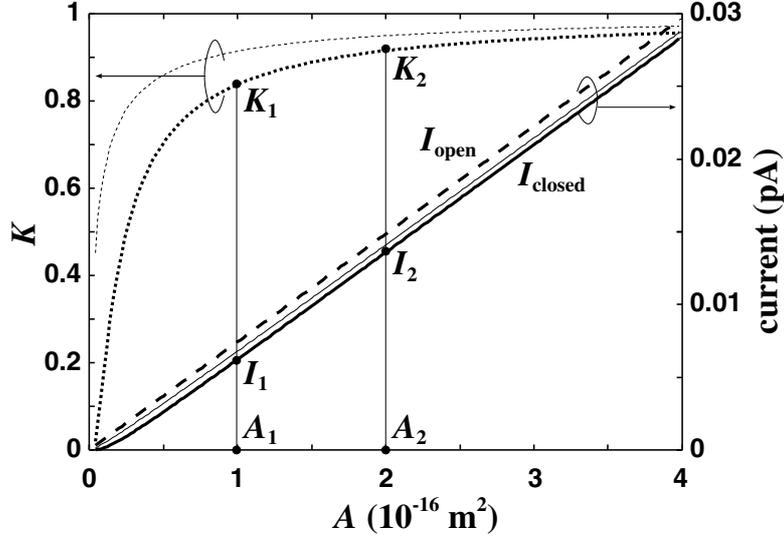
Figure 4. The thick solid and broken lines show the current (defined as jA) for the 'closed' and the 'open' junction, respectively. The thick dotted line shows $K = j_{closed}/j_{open}$. The ideal parallel-plate capacitor model is used for the thick lines. The thin solid and dotted lines represent counterparts for a worst-case estimate. $V_{eff} = 10$ mV.

layer due to surface Fermi-level pinning. For given net junction areas A_1 and A_2, one finds $I_2/I_1 = (K_2/K_1)(A_2/A_1)$. It might be possible to observe $K_2/K_1 > 1$ in the voltage-biased tunnel junctions at dimensions of $\sqrt{A} \sim 10^{-7}$ m, with $A_2/A_1 \sim 2$.

As noted above, A is the net area of the tunnel junction, and therefore the actual cross section of the device (pillar) is larger than A. However, it is, in principle, possible to evaluate the depletion length. We have performed a two-dimensional device simulation using Spicer's two-level model [15], assuming a surface-state density of 5×10^{12} cm^{-2}. The surface depletion length is calculated to be about 40 nm. Thus one could estimate A from the actual pillar size.

We have so far assumed the capacitance C to be given by $C = \epsilon_\infty \epsilon_0 A/d$. However, deviation from the parallel-plate capacitance, which is valid only if $\sqrt{A} \gg d$, cannot be neglected with the parameters suggested above. A numerical calculation that takes into account the exact structure of the device is required to obtain $\phi_c(x)$. Instead of using such a method, we evaluated the capacitance between two parallel square conductors embedded in a dielectric matrix with dielectric constant ϵ_∞, taking account of a fringing electric field at the edges. Then we used the C thus calculated in equations (2) and (3). The C calculated in this way is larger than that for a pillar structure, thereby giving a worst-case estimate. The results are shown in figure 4 by thin lines. The effect would become more pronounced if the barrier layer had an engineered profile [16], which also is realizable in the GaAs/Al$_y$Ga$_{1-y}$As/GaAs system.

In conclusion, we have shown that the current in a voltage-biased ultrasmall tunnel junction is scaled anomalously as the junction size is varied, due to the single-electron charging effect. We suggested a possible experiment with GaAs/Al$_y$Ga$_{1-y}$As/GaAs systems and presented a rough estimate of the size of the effect. Finally, we point out that no real system strictly follows the global rule because of the environmental impedance [17], which we have ignored. We also add that there are other effects (quantum size effect, Kondo effect, Fermi-edge singularity etc) that are known to be important at low temperatures. These may make the experiment much more involved. Rigorous treatment of such effects, however, is beyond the scope of this article.

Acknowledgments

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