Single-electron tunneling through an asymmetrical tunnel barrier

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Issues pertaining to single-electron tunneling through an asymmetrical tunnel barrier are discussed. A simple means of incorporating the change in the barrier shape accompanying a tunneling event into calculation of tunnel resistance is proposed. Simulation results show that directionality of tunneling through asymmetrical tunnel barriers is not as strong as reported previously, and that even an unphysical effect could arise if the barrier shape change is neglected.

1 Introduction

We developed a single-electronics simulator named ESS [1, 2]. It is capable of simulating circuits of arbitrary configuration consisting of tunnel junctions, capacitors and voltage sources. ESS includes support for tunnel junctions with Asymmetrical Tunnel Barriers (ATBs) [3–6]. It calculates tunneling rates through ATBs somewhat differently from what have been done conventionally.

In systems consisting of ultrasmall tunnel junctions and capacitors, single-electron charging effect manifests itself. Let us consider single-electron tunneling through a thick barrier in a double junction system (Fig. 1). When an electron tunnels through C_s, voltage of the central island changes substantially as shown in Figs. 1(a) and 1(b). In this kind of system, the validity of calculating transmission coefficients, or equivalently tunnel resistance from the initial barrier shape shown in Fig. 1(a) (or possibly from the final barrier shape of Fig. 1(b)) is questionable. Tunneling rates should be calculated taking the barrier shape change into account. In what follows we shall discuss how ATBs, or more generally thick tunnel barriers should be treated.

2 Method

To see how tunnel resistance should be calculated, we examine the normal single-electron tunneling through thin Symmetrical Tunnel Barriers (STBs), for it is also accompanied by changes in voltages of the electrodes. The single-electron tunneling rate Γ is given by the golden rule Eq. (1).

$$\Gamma = \frac{2\pi}{\hbar} \sum_{kk'\sigma} |T_{k'k}|^2 f(\omega_k)[1 - f(\omega_{k'})]\, \delta(\omega_{k'} - \omega_k + \Delta F), \tag{1}$$

where k' and k are the electron wave numbers of the two sides of the junction, σ is the spin of the tunneling electron, $T_{k'k}$ is the tunneling matrix element, $f(\omega_k)$ is the Fermi function and $\Delta F = F_\mathrm{f} - F_\mathrm{i}$ is the change in free energy associated with the tunneling. If the tunnel junction under consideration is a voltage-biased single junction, ΔF in Eq. (1) becomes $-eV$. In more complex circuits, $V_\mathrm{eff} = -\Delta F/e$ can be regarded as an effective bias voltage applied to the junction, which does not change throughout the tunneling event. Equation (1) can be rewritten in an integral form as

$$\begin{aligned} \Gamma &= 2 \cdot \frac{2\pi}{\hbar} |T|^2 D_\mathrm{L} D_\mathrm{R} \int \mathrm{d}\omega_k\, f(\omega_k)[1 - f(\omega_k - \Delta F)] \\ &= \frac{1}{e^2 R_\mathrm{T}} \frac{-\Delta F}{1 - \exp(\Delta F / k_\mathrm{B} T)}, \end{aligned} \tag{2}$$

where $|T|^2$ is the matrix element at the Fermi surface of the electrode metal, D_L and D_R are the electron densities of states, and $R_\mathrm{T}^{-1} = 4\pi e^2 |T|^2 D_\mathrm{L} D_\mathrm{R} / \hbar$. Here we assumed that $T_{k'k}$ does not vary substantially near the Fermi surface so that we can take the tunnel resistance R_T to be constant.

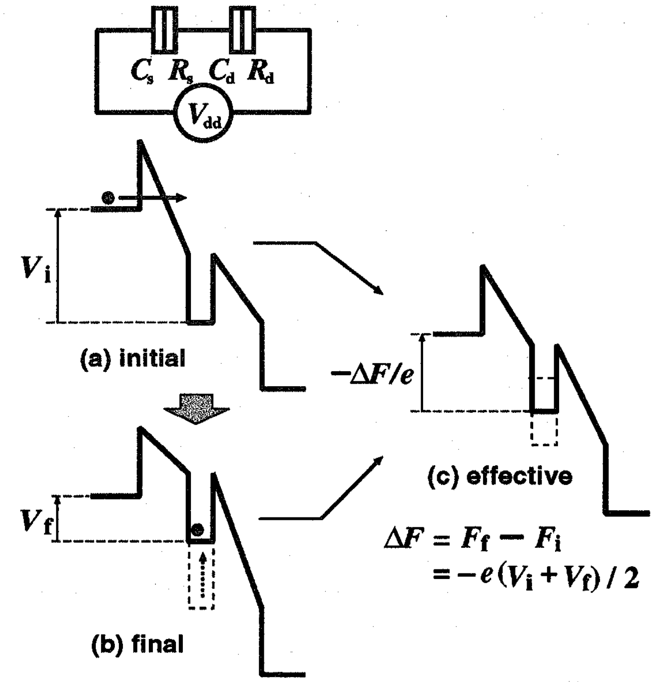

Fig. 1. Schematic potential barrier profiles of double junction circuit with thick tunnel barriers (a) before tunneling and (b) after tunneling. The voltages across tunnel junctions change substantially before and after tunneling due to single-electron charging effect. V_i is the voltage across the junction through which an electron tunnels before the tunneling event, and V_f is that after the tunneling event. (c) is the intermediate barrier shape used to calculate the tunneling rate.

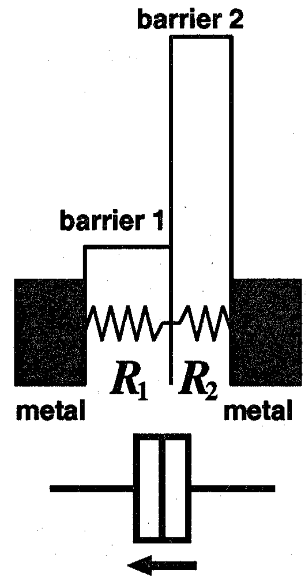

Fig. 2. Band diagram of bilayer ATB and its symbolic representation. R_1 and R_2 are the tunnel resistances of the component layers. Tunneling in the left direction is the forward tunneling.

This is a good approximation if ΔF is much smaller than the Fermi energy and the barrier height, and the barrier thickness does not change throughout tunneling.

As regards single-electron tunneling through an ATB, the barrier shape, especially the thickness, depends sensitively on the applied voltage. In order to incorporate the barrier shape change into the calculation of tunnel resistance, one should consider an effective barrier shape defined by the effective bias voltage $V_{\rm eff} = -\Delta F/e$ as is done in the case of single-electron tunneling through a thin STB. The resulting barrier shape is shown in Fig. 1(c). Contributions from the initial shape (Fig. 1(a)) and the final shape (Fig. 1(b)) are thus included in the effective barrier shape because ΔF can be written in terms of V_i and V_f as $\Delta F = -e(V_i + V_f)/2$. One should use this intermediate barrier shape to calculate the tunnel resistance.

3 Simulation Results

Bilayer ATBs shown in Fig. 2 are used in our simulation. It is composed of a thick insulator with a low barrier and a thin insulator with a high barrier [3, 5]. Here we use a simple resistor model for the bilayer ATBs [3]. When a forward bias voltage higher than a certain threshold V_t is applied, the tunnel resistance becomes R_2. Otherwise it is $R_1 + R_2$.

Shown in Fig. 3 is a single-electron transistor with an ATB. A similar circuit was studied by Nakashima and Uozumi using a more elaborate model than the resistor model [6]. They, however, did not take the barrier shape change into consideration when calculating transmission coefficients. They used the initial barrier shape for the calculation. Current-voltage curves of the transistor are computed using ESS in the two ways (Fig. 4). If the bias voltage applied to the ATB junction is

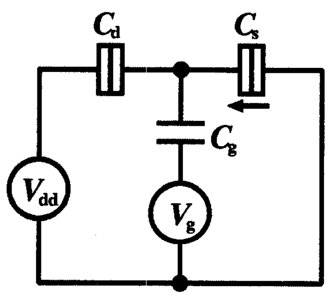

Fig. 3. Single-electron transistor with an ATB junction.

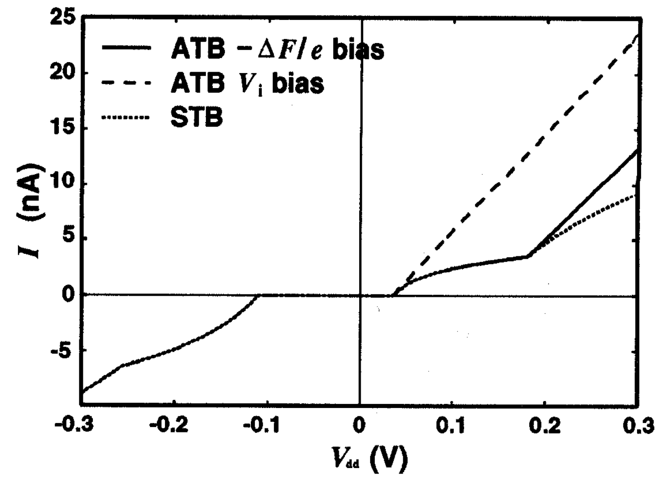

Fig. 4. Current-voltage curves of the single-electron transistor shown in Fig. 3. Tunneling rates are calculated from the intermediate shape (solid line) and the initial shape (dashed line). Result for a normal single-electron transistor consisting of STBs is also shown for comparison (dotted line). $C_d = C_s = 0.1\,\text{aF}$, $C_g = 1\,\text{aF}$, $R_d = R_{s1} + R_{s2} = 10\,\text{M}\Omega$, $R_{s2} = 100\,\text{k}\Omega$, $V_g = 0.6\,\text{V}$, $V_t = 78\,\text{mV}$ and $T = 4.2\,\text{K}$.

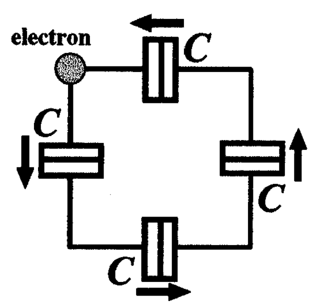

Fig. 5. Loop of ATB junctions. An extra electron is placed onto the circuit. Every node has self-capacitance but is not drawn for simplicity.

taken to be V_i, directionality of the transistor is pronounced. If V_{eff} is used, the current-voltage curve is more similar to that of the normal single-electron transistor, which consists of thin STBs, within a low voltage range.

Our results indicate that the directionality of tunneling through an ATB is not as strong as expected from the barrier shape before tunneling. For quantitative discussion, the oversimplified resistor model is insufficient. Nevertheless, we would like to emphasize the significance of the use of V_{eff}. Next, we shall give an example in which it makes a qualitative difference which barrier shape is used in the calculation of tunnel resistance.

Kanaami et al. brought up an intriguing question pertinent to ATBs [7]. What would happen if ATBs are connected circularly and an extra electron is placed onto the circuit as shown in Fig. 5? Is there a possibility of observing circular thermal tunnel current rectified by ATBs? As for the tunneling of the extra electron, ΔF is always zero, which means that there is no driving force for tunneling that originates from electrostatic energy. Tunnel current flows due to finite temperature.

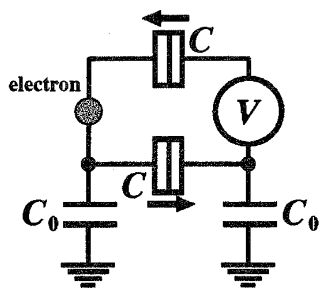

Fig. 6. Loop of two ATB junctions with an extra electron.

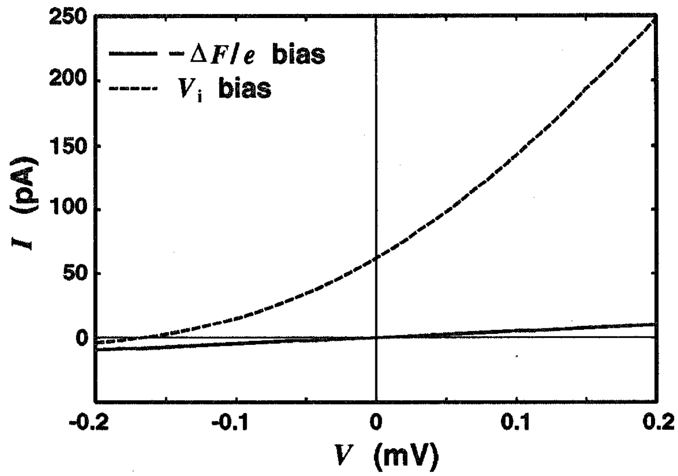

Fig. 7. Current in the loop circuit shown in Fig. 6. Tunneling rates are calculated from intermediate barrier shapes (solid line) and initial barrier shapes (dashed line). $C = C_0 = 10\,\mathrm{aF}$, $R_1 + R_2 = 5\,\mathrm{M}\Omega$, $R_2 = 200\,\mathrm{k}\Omega$, $V_t = 3\,\mathrm{mV}$ and $T = 0.3\,\mathrm{K}$.

The two-junction circuit shown in Fig. 6 is good enough for studying the loop circuit. Simulation results are shown in Fig. 7. The current at $V = 0$ is of our concern. When tunnel resistance is determined by the initial barrier shape, circular zero-bias current is observed. By contrast, when the effective barrier shape is used instead, the effective bias voltage applied to the junctions is zero as long as $V = 0$. It follows that the tunnel resistances are the same irrespective of the tunneling direction of the extra electron; i.e. the reverse tunneling rate through the upper junction and the forward tunneling rate through the lower junction (Fig. 6) are the same. Net tunnel current, therefore, is zero. This exemplifies the significance of incorporating the barrier shape change.

In conclusion, I-V curves for a voltage-biased single tunnel junction should be regarded as I-V_{eff} curves in more complex circuits. The use of the effective barrier shape as defined by $V_{\mathrm{eff}} = -\Delta F/e$ is more valid in physical respect than to use the barrier shape before tunneling. The latter implies that characteristics of a junction change when it becomes a component of a circuit, which is unacceptable.

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