Effect of the Tunneling Rates on the Conductance Characteristics of Single-Electron Transistors

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Abstract

We present calculations of the linear-response conductance of a SiGe based single-electron transistor (SET). The tunneling rates through the source- and lead barriers are calculated using Bardeen's transfer Hamiltonian formalism [4]. The tunneling matrix elements are calculated for transitions between the 0D states in the quantum dot and the lowest subband in the 1D constriction. We compare the results for the conductance peaks with those from calculations with a constant rate, i. e. where the shape of the peaks is only due to energetic arguments.

1 Introduction

Single-electron tunneling in semiconductor nanodevices such as single-electron transistors is an interesting subject for application-oriented research towards new device principles. Even

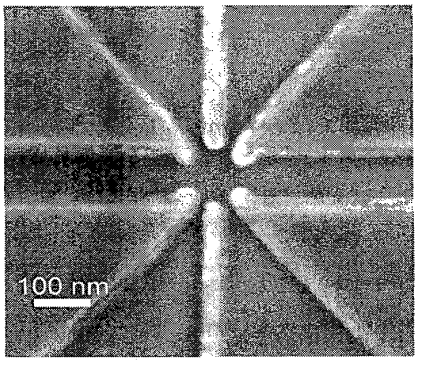

Figure 1: *Top view of the metallic gates of the SET.*

though an ever increasing number of SET structures showing clear signs of single-electron tunneling combined with Coulomb-blockade (CB) are now available, the interpretation of peak spacings and peak heights of the CB peaks is still controversial. Main issues concerning for instance the statistics of the peak spacing still remain unresolved (for recent work see [1] and [2]). Most of the analysis of experimental data is carried out using the so-called *orthodox theory* of CB and its extensions towards semiconductor structures, the *constant interaction model* (CI) for the dot states. The basic assumptions of this theory allow to predict the main trends in the line shape and the peak height as well as the spacing of the CB peaks within certain regimes which are given by the range of the dot level spacing, $\Delta\epsilon$, and the thermal energy, $k_{\mathrm{B}}T$ [3]. The basis of this analysis is an equation for the linear-response current of a quantum dot connected to a reservoir via two tunneling barriers

$$G = \frac{e^2}{k_{\mathrm{B}}T} \sum_{\{n_i\}} P_{\mathrm{eq}}(\{n_i\}) \sum_k \delta_{n_k,0} \frac{\Gamma_k^{\mathrm{s}} \Gamma_k^{\mathrm{d}}}{\Gamma_k^{\mathrm{s}} + \Gamma_k^{\mathrm{d}}} f(F(\{n_i + k\}, N+1) - F(\{n_i\}, N) - E_{\mathrm{F}}), \quad (1)$$

$F(\{n_i\}, N)$ is the total free energy of the system with N electrons in the quantum dot and the occupation configuration $\{n_i\}$, $n = 0, 1$, where E_F is the Fermi energy and $P_{eq}(\{n_i\})$ is the Gibbs distribution function of the electron population of a quantum dot in equilibrium with the reservoirs. Γ^d and Γ^s are the tunneling rates for the drain- and source-side barrier. The tunneling rates are often assumed to be constant or just to depend on the width of the barrier. Such a treatment is only able to reveal the effect of the free energies on both line shape and peak hight of the conductance peaks. In this paper we present calculations of the tunneling rates using Bardeen's *transfer Hamiltonian* formalism [4]. The tunneling rates are inserted into Eq. (1) and the effects of the tunneling rates on the heights of the CB peaks are investigated for a Si test structure.

2 Bardeen's transfer Hamiltonian formalism

We straightforwardly apply the transfer Hamiltonian formalism given in [4] and [5] to a reservoir/dot system, where the dot is separated from the reservoir by two narrow quasi-1D channels (leads). By applying a voltage to an electrostatic gate above the channel we create a narrow constriction (Fig. 2). We assume that the width of the constriction in its center allows only one transverse state below the Fermi level [6]. Therefore, the constriction can be

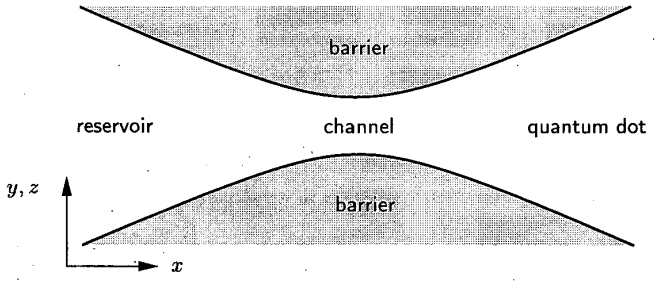

Figure 2: *(a) Schematic view at the constriction.*

considered a quantum-point contact separating the dot and the reservoir. The wave function of a state penetrating the constriction (but still outside the barrier) is one-dimensional

$$\Psi(x, y, z) = \phi_0(x; y, z)e^{ikx} \tag{2}$$

assuming the quasi-1D channel to extend along the x-direction. $\phi_0(x; y, z)$ is the wave function for the transverse motion and k denotes the associated wavevector. Within the barrier the wavefunction is treated in the WKB approximation

$$\Psi(x, y, z) = \phi_0(x; y, z)e^{w(x)}, \quad w(x) = \int_a^x dx' \kappa(x'), \tag{3}$$

with the WKB wavevector given by $(\hbar^2/2m_\perp^*)\kappa^2(x) = E_0 - V(x)$. E_0 is the energy of the transverse mode, V the barrier potential, a is the classical turning point in the lead and $W(x) = \exp[w(x)]$ is called the barrier-penetration factor. With these assumptions the matrix element for the transition from the lowest transverse state ϕ_0 in the constriction to the kth dot state ψ_k can be approximated by

$$M_k \approx -\frac{\hbar^2}{2m_\parallel^*} W(x_b) \iint\limits_{\partial\Omega(y,z)} \mathrm{d}y\, \mathrm{d}z\, \phi_0(x_b; y, z) \left[\kappa(x_b)\psi_k(x_b; y, z) - \frac{\partial}{\partial x}\psi_k(x_b; y, z)\right]. \tag{4}$$

The tunneling rate for this transition is then given as

$$\hbar\Gamma_k = 2\pi |M_k|^2 \delta(E_0 - \epsilon_k). \tag{5}$$

We calculate the eigenvalue spectrum of the quantum dot self-consistently by solving a nonlinear Schrödinger/Poisson equation on a 3D mesh comprising the dot area as well as the barrier regions [7]. The wavefunction for the transverse mode ϕ_0 in the constriction is obtained as the solution of the Schrödinger/Poisson equation solving the Schrödinger equation in slices along the 1D-channel in the leads. The wavefunctions are then used to evaluate the matrix element, Eq. (4), and the tunneling rate, Eq. (5). Finally, the conductance is obtained from Eq. (1).

3 Results

Fig. 3 shows the dependence of the conductance peaks on the tunneling rates. In the upper panel, the tunneling rates in the conductance formula Eq. (1) were kept at a constant value of $\Gamma_k = 1s^{-1}$ for all k. In the lower panel, the tunneling rates were explicitly calculated

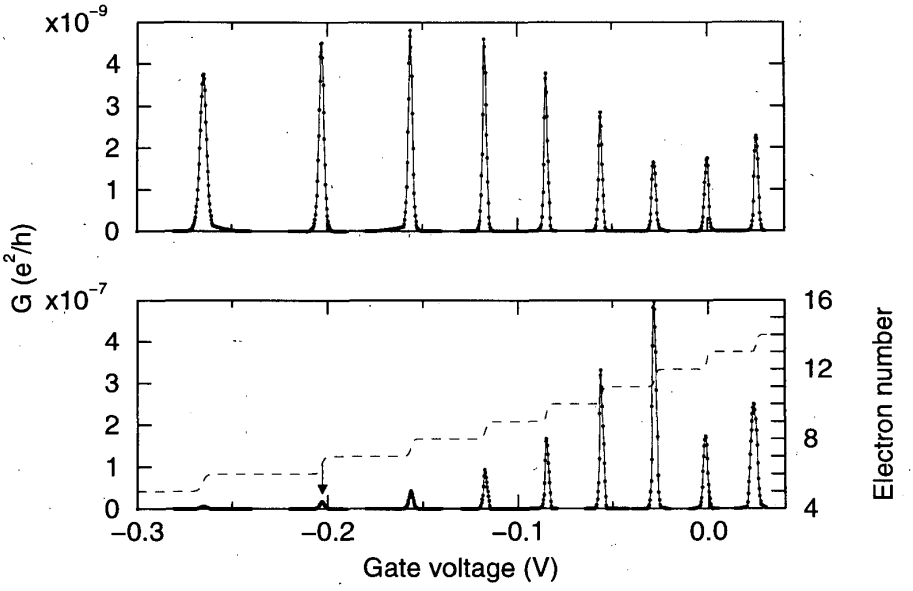

Figure 3: *Upper panel: conductance peaks for a constant tunneling rate* $\Gamma_k = 1s^{-1}$ *for all dot levels. Lower panel: conductance peaks calculated with tunneling rates according to Eqs. (4, 5). Dashed line: charging of the quantum dot.*

using the formalism described above. We see a strong suppression of the first up to the fifth peak. The inset shows one particular conductance peak from the lower panel in comparison to the corresponding peak from the upper panel, however, scaled to the same peak height. It can be seen that even though the peak height is different, the shape of the peak remains the same. Therefore it can be concluded that the principal shape of the conductance peak is not altered by the inclusion of realistic tunneling rates. i.e. the shape of the conductance peaks is soleley determined by the temperature dependent distribution of the electrons in the quantum dot and not by the energetic barrier.

4 Summary

We showed that the inclusion of realistic tunneling rates within the linear-response conductance formula of Beenakker [3] severely alters the results for the conductance characteristics of a single-electron transistor. While the line shape scaled to the same peak hight remains the

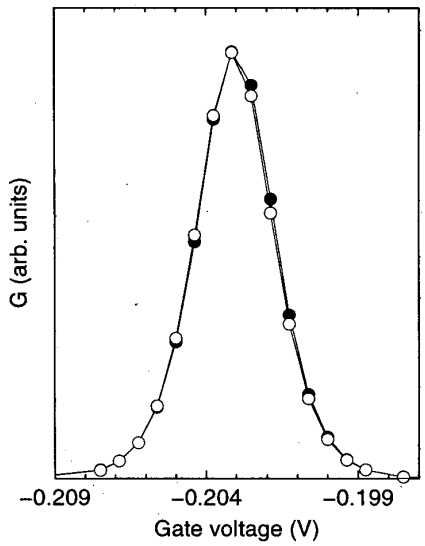

Figure 4: *The marked conductance peak from the lower panel in Fig. 3 overlaid by the corresponding peak from the upper panel.*

same, some of the peaks, especially at the lower end of the spectrum get almost completely suppressed. This effect is due to the low energy of those eigenvalues which contribute to the tunneling rate (at low temperatures this is only one level), and therefore the much wider barrier these electrons have to traverse in the tunneling process. This result is in qualitative agreement with many experimental findings (see for instance [8]).

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