Self consistent charge-current in a mesoscopic region attached to superconductor leads

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Abstract

We investigate the behavior of a electric potential profile inside a mesoscopic region attached to a pair of superconducting leads. It turns out that $\mathrm{I}-V$ characteristic curves are strongly modified by this profile. In addition, the electronic population in the mesoscopic region is affected by the profile behavior. We discuss the single particle current and the mesoscopic electronic population within the non-equilibrium Keldysh Green functions technique. The Keldysh technique results are further converted in a self consistent field (SFC) problem by introducing potential profile modifications as proposed by Datta. Evaluation of $\mathrm{I}-V$ characteristics are presented for several values of the model parameters and comparison with current experimental results are discussed.

1 Introduction

Usual mesoscopic devices consist of a mesoscopic region coupled to a pair of macroscopic contacts or leads (source and drain) which are in thermodynamic equilibrium. By applying a source voltage V_s and a drain voltage V_d an electric current can flow between the leads and across the mesoscopic region which sets a typical non equilibrium situation. Besides the applied drain voltages V_d and source voltage V_s the system is further manipulated by a gate voltage V_g which, in principle, couples directly to the mesoscopic region. It turns out that V_d, V_s and V_g induce an effective electrostatic profile potential inside the mesoscopic region in such way that electronic population and electric current become tied to a self consistent problem. It is quite clear since such potential profile modifies the mesoscopic region level structure in a self consistent fashion. Such situation can be highly complicated since it mixes non equilibrium statistical mechanics with a classic electrostatic framework. Here, we adopt a simple approach put forward by Datta [1] which relates the self consistent electrostatic profile to the electronic population of the mesoscopic region and to the electric current. Datta original approach considers a pair of macroscopic leads in the normal state such that our model could be considered a generalization to the case of superconducting leads. The self consistency and any other model calculations are fully performed within the non equilibrium Keldysh technique [2, 3].

In section 2 we discuss a mesoscopic region which describes a single quantum dot whith a spin degenerated level coupled to superconductors leads . In addition, we show calculations which lead to a self consistent field (SFC) problem between dot electronic population and electric current between the superconducting leads. The self consistency takes into account electric potential profiles inside the mesoscopic region as induced by the drain and source bias and by the gate voltage [1].

In section 3 we present our results about the effect of the potential profile on the $I-V$ characteristic curves and on the electronic population inside the mesoscopic region.

Finally, in section 4 we discuss our main conclussions.

2 Model and formulation

In this section we present the model and calculations wich lead to the current and to the population number in the mesoscopic region. We want to point out that it is evaluated under a single widely used approximation: The wide band limit (WBL) of the superconducting leads. The results are still valid when the real part of left lead (L) and right lead (R) self energies do not vanish out.

We consider a spin degenerated single orbital in a quantum dot connected to superconductors leads [4, 5]. The hamiltonian which describes this system is a generalized Friedel-Anderson model [6]. It reads

$$H = H_S + H_D + H_T, \tag{1}$$

where H_S, H_D and H_T stand for the superconducting leads, the dot and the tunneling term, respectively. $H_S = H_L + H_R$ where H_L and H_R are the left and right lead hamiltonians, respectively. They are given, within the BCS model [7], by

$$H_\eta = \frac{{\Delta_\eta}^2}{v_\eta} + \sum_{\vec{k}\sigma} \epsilon_{\eta\vec{k}} a^\dagger_{\eta\vec{k}\sigma} a_{\eta\vec{k}\sigma} - \frac{1}{2}\Delta_\eta \sum_{\vec{k}\sigma} \sigma \left(a^\dagger_{\eta\vec{k}\sigma} a^\dagger_{\eta-\vec{k}-\sigma} + a_{\eta-\vec{k}-\sigma} a_{\eta-\vec{k}-\sigma} \right), \tag{2}$$

where Δ_η and v_η are the superconductor gap and the BCS coupling constant, respectively, of the lead $\eta = L, R$. H_D is the hamiltonian for the quantum dot single-level of energy ε:

$$H_D = \varepsilon \sum_\sigma d^\dagger_\sigma d_\sigma. \tag{3}$$

The tunneling hamiltonian H_T reads

$$H_T = \sum_\eta V_\eta \sum_{\vec{k}\sigma} \left(a^\dagger_{\eta\vec{k}\sigma} d_\sigma + d^\dagger_\sigma a_{\eta\vec{k}\sigma} \right). \tag{4}$$

H_T connects the dot to the biased superconducting leads and it allows the electric charge flux.

The flow of electric charge from the terminal η is given by

$$\mathrm{I}_\eta\,(t) = (-e)\left[-\frac{d\langle N_\eta(t)\rangle}{dt} \right] = \frac{\mathrm{i}e}{\hbar}\langle [H_T(t), N_\eta(t)]\rangle, \tag{5}$$

where $-\mathrm{e}$ is the electron charge. $\langle\cdots\rangle$ is the thermodynamical average over the L and R leads which are maintained at chemical potentials μ_L y μ_R, respectively. $eV = \mu_L - \mu_R$. V is the electric potential difference between the leads. Later on we will single out, from equation (5), the single particle electric current. Equation (5) can be expressed in terms of the ordered Keldysh Green function

$$\mathrm{F}_{\eta\vec{k}\sigma}(t, t') \equiv -\mathrm{i}\langle \mathrm{T_c} a_{\eta\vec{k}\sigma}(t) d^\dagger_\sigma(t')\rangle \tag{6}$$

as

$$\mathrm{I}_\eta\,(t) = \frac{2e}{\hbar} V_\eta \Re \sum_{\vec{k}\sigma} \mathrm{F}^{<}_{\eta\vec{k}\sigma}(t,t), \tag{7}$$

where $\mathrm{F}^{<}_{\eta\vec{k}\sigma}(t,t')$ is a lesser Keldysh Green function. In order to evaluate $\mathrm{F}^{<}_{\eta\vec{k}\sigma}(t,t')$ we set an equation of motion for the ordered Keldysh Green function $\mathrm{F}_{\eta\vec{k}\sigma}(t,t')$. It turns out that the $\mathrm{F}_{\eta\vec{k}\sigma}(t,t')$ contribution to the single particle current becomes coupled to the dot Keldysh Green function

$$\mathrm{G}_\sigma(t,t') = -\mathrm{i}\langle \mathrm{T_c} d_\sigma(t) d^\dagger_\sigma(t')\rangle \tag{8}$$

Such relation can be expressed as an integral equation over the Keldysh contourn C_K:

$$\mathrm{F}_{\eta\vec{k}\sigma}(t,t') = \int_{C_K} dt''\, \mathrm{g}_{\eta\vec{k}}\,(t,t'')\, \mathrm{G}_\sigma\,(t'',t') \tag{9}$$

where $\mathrm{g}_{\eta\vec{k}}\,(t,t') = -\mathrm{i}\left\langle \mathrm{T_c}\, a_{\eta\vec{k}\sigma}\,(t)\, a^\dagger_{\eta\vec{k}\sigma}\,(t')\right\rangle_0$ is the unperturbed Keldysh Green function of lead $\eta = L, R$. The subscript $_0$ indicates that its evaluation ocurrs with $V_\eta = 0$. By using Langreth rules [8], $\mathrm{F}^{<}_{\eta\vec{k}\sigma}(t,t')$ can be written as an integral equation along the real axis

$$\mathrm{F}^{<}_{\eta\vec{k}\sigma}(t,t') = \int_{-\infty}^{\infty} \mathrm{d}t'' \left[\mathrm{g}^{(\mathrm{r})}_{\eta\vec{k}}\,(t,t'')\, \mathrm{G}^{<}_\sigma\,(t'',t') + \mathrm{g}^{<}_{\eta\vec{k}}\,(t,t'')\, \mathrm{G}^{(\mathrm{a})}_\sigma\,(t'',t')\right] \tag{10}$$

$^{(\mathrm{a})}$ and $^{(\mathrm{r})}$ superscripts denote advanced and retarded Keldysh Green functions, respectively. $\mathrm{g}^{\overset{(\mathrm{r})}{<}}_{\eta\vec{k}}\,(t,t')$ depends on $t-t'$ and Fourier transform of $\mathrm{G}^{\overset{<}{(\mathrm{a})}}_\sigma\,(t,t')$ is $\propto \delta\,(\omega-\omega')$ such that the current becomes time independent.

By inserting expression (10) into (7), the single particle current I_η is found in terms of the dot Keldysh Green Function $\mathrm{G}_\sigma\,(t,t')$

$$\mathrm{I}_\eta \;=\; \frac{2e}{h} \Re \sum_\sigma \int_{-\infty}^{\infty} \mathrm{d}\omega \left[\Sigma^{(\mathrm{r})}_\eta\,(\omega)\, \mathrm{G}^{<}_\sigma\,(\omega) + \Sigma^{<}_\eta\,(\omega)\, \mathrm{G}^{(\mathrm{a})}_\sigma\,(\omega)\right], \tag{11}$$

$\Sigma^{\overset{(\mathrm{r})}{<}}_\eta\,(\omega)$ are Keldysh self energies which are given by

$$\Sigma^{\overset{(\mathrm{r})}{<}}_\eta\,(\omega) = V_\eta^2 \sum_{\vec{k}} \mathrm{g}^{\overset{(\mathrm{r})}{<}}_{\eta\vec{k}}\,(\omega) \tag{12}$$

They are trivially evaluated since they just involve thermodynamical averages over isolated superconducting leads:

$$\begin{aligned}
\Sigma_\eta^{(\mathrm{r})}(\omega) &= -\Gamma_\eta \left[\frac{\omega-\mu_\eta}{\Delta_\eta}\rho_s\left(\Delta_\eta,\omega-\mu_\eta\right)+\mathrm{i}\rho_s\left(\omega-\mu_\eta,\Delta_\eta\right)\right], \\
\Sigma_\eta^{<}(\omega) &= 2\mathrm{i}\Gamma_\eta\rho_s\left(\omega-\mu_\eta,\Delta_\eta\right)\mathrm{f}\left(\omega-\mu_\eta\right), \\
\rho_s\left(\omega,\omega'\right) &\equiv \Theta(|\omega|-|\omega'|)\frac{|\omega|}{\sqrt{\omega^2-\omega'^2}}.
\end{aligned}$$

$\Gamma_\eta = \pi N_\eta\left(\omega-\mu_\eta\right)V_\eta^2 \approx \pi N_\eta(0)\,V_\eta^2$ are the coupling constants between the leads and the quantum dot in the WBL. $N_\eta(0)$ is the density of states at the η Fermi level and $\mathrm{f}(\omega)$ is the Fermi-Dirac distribution function.

Similarly, the Keldysh Green function $\mathrm{G}_\sigma(t,t')$ is determined from the equation of motion technique and we just show the final result for the single particle current

$$\mathrm{I} = \frac{4e}{h}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\frac{\Gamma_L(\omega-eV)\,\Gamma_R(\omega)}{\Gamma_L(\omega-eV)+\Gamma_R(\omega)}\,\rho(\omega)\left[\mathrm{f}(\omega-eV)-\mathrm{f}(\omega)\right], \tag{13}$$

In (13) we performed a trivial shift of the dot energy level and insert the electric potencial V through $eV=\mu_L-\mu_R$. $\Gamma_\eta(\omega)$ and $\rho(\omega)$ are given by

$$\begin{aligned}
\Gamma_\eta(\omega) &= \Gamma_\eta\rho_s\left(\omega,\Delta_\eta\right) &(14)\\
\rho(\omega) &= \sum_\sigma\left(-\frac{1}{\pi}\right)\Im\mathrm{G}_\sigma^{(\mathrm{r})}(\omega) = 2\,\frac{\Gamma(\omega)/\pi}{(\omega-\varepsilon)^2+\Gamma^2(\omega)} &(15)\\
\Gamma(\omega) &= \Gamma_L(\omega-eV)+\Gamma_R(\omega) &(16)
\end{aligned}$$

Here $\rho(\omega)$ is the so-called quantum dot spectral function which is given in terms of the retarded $\mathrm{G}^{(\mathrm{r})}(\omega)$ Keldysh Green function [2]. At steady state there is no net flux into or out of the mesoscopic channel which yields a stationary particle number in it. The population number N, at the dot, is given by

$$N = 2\left[-\mathrm{i}\mathrm{G}^{<}(t,t)\right] = 2\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\,\mathrm{G}^{<}(\omega), \tag{17}$$

which becomes a weighted average over the L and R contacts

$$N = 2\int_{-\infty}^{\infty}\mathrm{d}\omega\,\rho(\omega)\left[\frac{\Gamma_L(\omega-eV)}{\Gamma(\omega)}\,\mathrm{f}(\omega-eV)+\frac{\Gamma_R(\omega)}{\Gamma(\omega)}\,\mathrm{f}(\omega)\right]. \tag{18}$$

So far we are not included the side effects of a potential profile inside the mesoscopic channel. Such potential is induced by the action of source and drain bias applied voltages and from the action of the gate voltage. The potential profile effect has been studied by Datta [1] on a channel attached to simple normal leads. Datta found that $I-V$ characteristics are affected by the self consistent potential U inside the channel and pointed out its importance in addressing the correct position of the mesoscopic single energy level. Within the Datta approach [1], U is given by

$$U = U_{\mathcal{L}} + \frac{e^2}{C_E}\,\Delta N \tag{19}$$

$U_{\mathcal{L}}$ is the Laplacian potential which ignores the electronic population. The interesting term is the second one which introduces the dependence on the electronic population N. $\Delta N = N - N_0$. N_0 is the electronic population when $V = 0$. $U_0 = e^2/C_E$ is the dot charging energy. C_E is an effective dot capacitance which depends on drain C_D, source C_S and gate C_G capacitances within an equivalent circuit framework. Indeed, $U_{\mathcal{L}}$ can be included in the unperturbed single energy level ε. Therefore it turns out that whenever we take into account the potential profile inside the mesoscopic channel, it amounts to a shift of the single dot level by $U = e^2\Delta N/C_E$. It is equivalent to the replacement of $\rho\left(\omega\right)$ by $\rho\left(\omega - U\right)$ in the current and electronic population evaluation which becomes a self consistent field (SFC) problem.

Finally, the self consistent equations for the single particle electric current and the electronic population are given by

$$\mathrm{I} = \frac{4e}{h}\int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\Gamma_L\left(\omega - eV\right)\Gamma_R\left(\omega\right)}{\Gamma_L\left(\omega - eV\right) + \Gamma_R\left(\omega\right)}\,\rho\left(\omega - U\right)\left[\mathrm{f}\left(\omega - eV\right) - \mathrm{f}\left(\omega\right)\right], \tag{20}$$

$$N = 2\int_{-\infty}^{\infty} \mathrm{d}\omega\,\rho\left(\omega - U\right)\left[\frac{\Gamma_L\left(\omega - eV\right)}{\Gamma\left(\omega\right)}\,\mathrm{f}\left(\omega - eV\right) + \frac{\Gamma_R\left(\omega\right)}{\Gamma\left(\omega\right)}\,\mathrm{f}\left(\omega\right)\right]. \tag{21}$$

Equation (21) determines N in a self consistent fashion which inmediately yields the electric current I by carrying out the integration in (20).

We will consider a situation where the lead couplings are not extremely small and the dot capacitance is reasonably large. It will smear out the Coulomb blockade effect and the double occupancy of the resonant level will be very unlikely.

3 Results

In 1 and 2 we show zero temperature I-V characteristics, for values of gate voltage $V_g > 0$ and $V_g < 0$ respectively. As we can see in 2, the current is nonzero for positive values of the drain voltage, while for negative values of the drain voltage the current vanishes out. For 3 the current is nonzero for negative values of the drain voltage, while there is no current for positive values of the drain voltage.

In 3 and 4 we show zero temperature I-V characteristics as calculated with Datta self consistent method, for values of gate voltage $V_g > 0$ and $V_g < 0$ respectively. In this case we can observe that the current shows a symmetry for positive and negative values of the gate voltage.

Furthermore, it is noted that the graphs agree with experimental data reported in the literature [9].

4 Conclusions

In conclusion, we have studied a mesoscopic region which describes a spin degenerated single quantum dot coupled to superconductors leads, whenever the Coulomb blockade is neglected, in the regime $\Delta \gg \Gamma_{L,R}$. We derived an exact electric current within non equilibrium Keldysh technique. In addittion zero temperature $I - V$ characteristics agree with the experimental results. Furthermore, we showed there are symmetric I-V characteristic, within the self consistent method for the potential profile.

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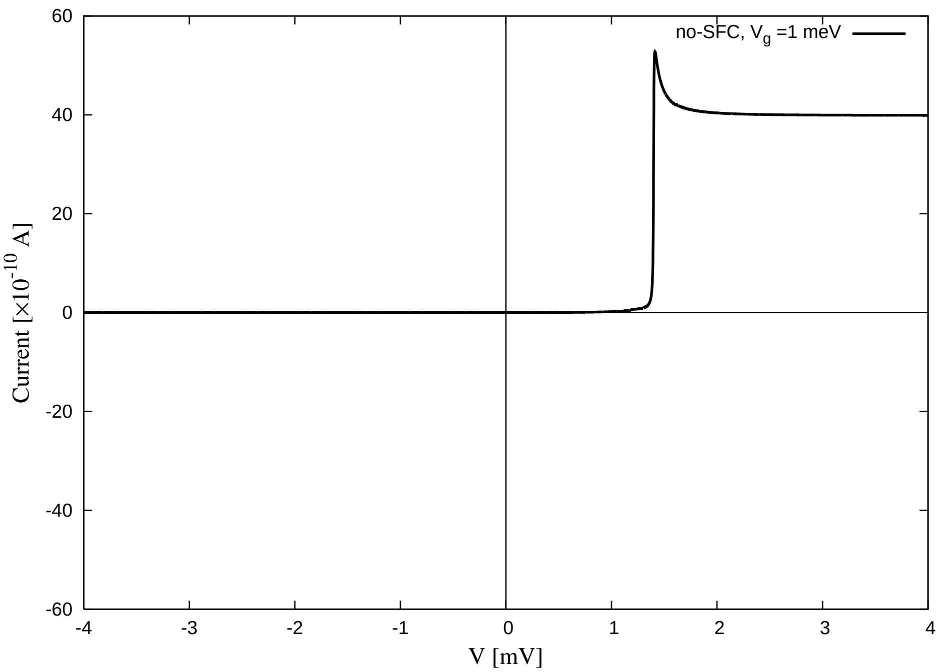

Figure 1: Zero temperature I-V characteristics calculated without the use self consistent field (no-SFC) method, with $\varepsilon = 0.2$ meV, $V_g = 1$ meV, $U_0 = 0.0025$ meV, $C_D/C_E = 0.5$, $\Gamma_L = \Gamma_R = 0.008$ meV and $\Delta = 0.2$ meV.

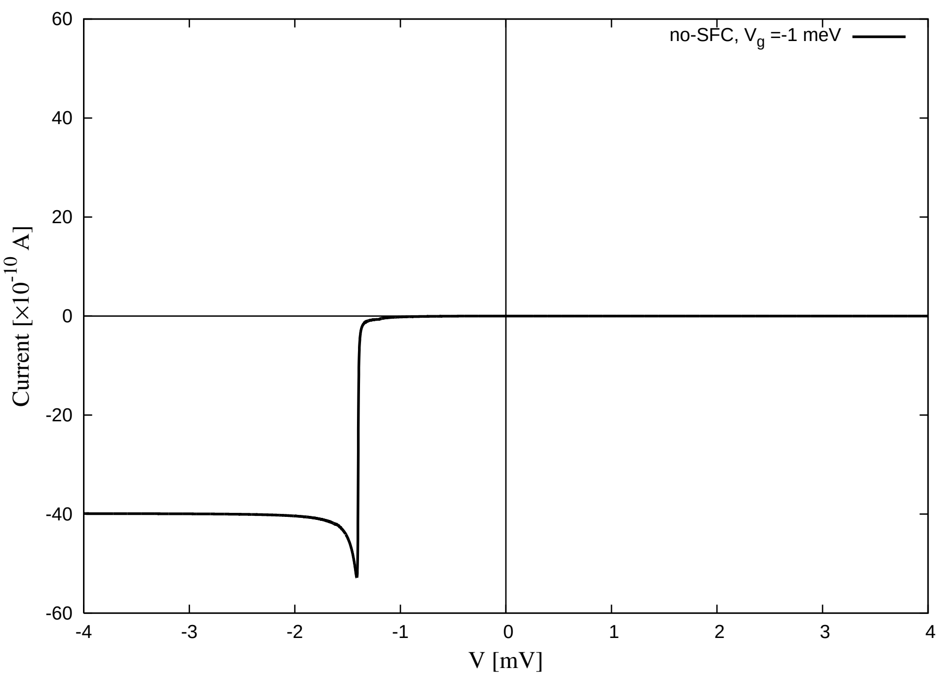

Figure 2: Zero temperature I-V characteristics calculated without the use self consistent field (no-SFC) method, with $\varepsilon = 0.2$ meV, $V_g = -1$ meV, $U_0 = 0.0025$ meV, $C_D/C_E = 0.5$, $\Gamma_L = \Gamma_R = 0.008$ meV and $\Delta = 0.2$ meV.

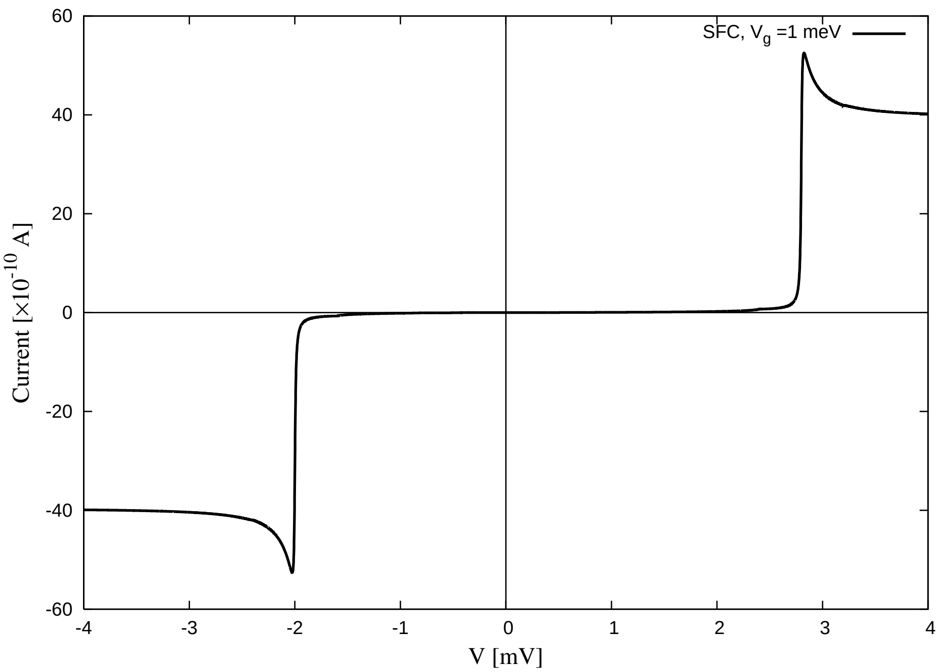

Figure 3: Zero temperature I-V characteristics calculated using the self consistent field (SCF) method, with $\varepsilon = 0.2\,\text{meV}$, $V_g = 1\,\text{meV}$, $U_0 = 0.0025\,\text{meV}$, $C_D/C_E = 0.5$, $\Gamma_L = \Gamma_R = 0.008$ meV and $\Delta = 0.2$ meV.

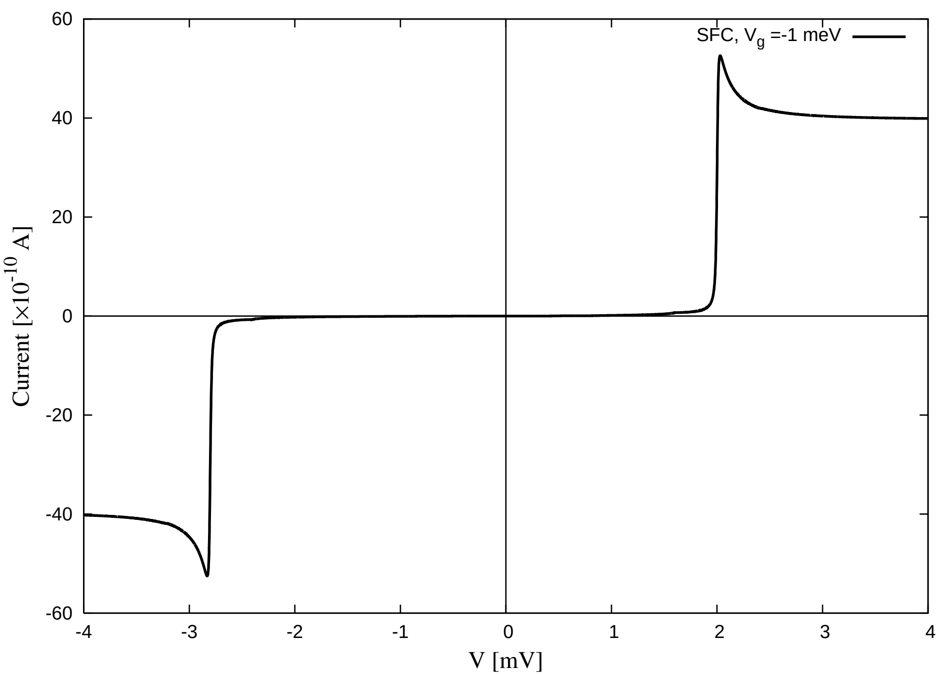

Figure 4: Zero temperature I-V characteristics calculated using the self consistent field (SCF) method, with $\varepsilon = 0.2$ meV, $V_g = -1$ meV, $U_0 = 0.0025$ meV, $C_D/C_E = 0.5$, $\Gamma_L = \Gamma_R = 0.008$ meV and $\Delta = 0.2$ meV.