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

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Abstract

We investigate the behavior of an electric potential profile inside a mesoscopic region attached to a pair of superconducting leads. It turns out that the $I-V$ characteristic curves are strongly modified by this profile. In addition, the electronic population in the mesoscopic region is affected by the profile behavior. We derive 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 (SCF) problem by introducing potential profile modifications. Evaluation of $I-V$ characteristics are presented for several values of the model parameters and comparison with current experimental results are discussed.

Keywords: Quantum dot, Superconductors, Keldysh Green Functions

1. Introduction

From the demonstration of a superconductor-normal-superconductor (S-N-S) transistor [1], the study of the nonequilibrium transport through superconducting systems has been of much interest [2, 3, 4, 5, 6]. Another interesting problem in mesoscopic physics is transport through a superconductor/quantum dots/superconductor system [7, 8, 9, 10, 11, 12, 13, 14, 15]. In this paper, we study the effect of an electrostatic potential profile on the electric transport across a single quantum dot with a spin degenerated level. Such a dot is coupled to a pair of biased superconductors contacts or leads (source and drain). By applying a source voltage $V_S$ and a drain voltage $V_D$ an electric current can flow between the leads and across the quantum dot 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 quantum dot. It turns out that $V_D$, $V_S$ and $V_G$
induce an effective electrostatic profile potential inside the mesoscopic region in such a way that electronic population and electric current become tied to a self consistent problem. It is quite clear that such potential profile modifies the quantum dot 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 an approach which relates the self consistent electrostatic profile to the electronic population of the quantum dot and to the electric current\cite{16,17}. The self consistency and any other model calculations are fully performed within the non equilibrium Keldysh technique\cite{18,19}.

In section\textbf{2} we find the expression for the current and the electronic population for a mesoscopic region. In addition, we show calculations which lead to a self consistent field (SCF) problem between the dot electronic population and the 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\cite{17}. Moreover we present the 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\textbf{4} we discuss our main conclusions.

\section{Calculation}

In this section we present the model and calculations which lead to the current and to the population number in the mesoscopic region.

We consider a spin degenerated single orbital in a quantum dot connected to superconductors leads. The hamiltonian which describes this system is a generalized Friedel-Anderson model\cite{20}. It reads

$$H = H_S + H_D + H_T,$$

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\cite{21}, by

$$H_S = \sum_{\eta\vec{k}\sigma} \Psi_{\eta\vec{k}\sigma}^\dagger H_{\eta\vec{k}}^0 \Psi_{\eta\vec{k}\sigma},$$

with

$$H_{\eta\vec{k}}^0 = \begin{pmatrix} \varepsilon_{\eta\vec{k}} & \Delta_{\eta-\vec{k}} \\ \Delta_{\eta\vec{k}}^* & -\varepsilon_{\eta\vec{k}} \end{pmatrix},$$

where $\Delta_{\eta\vec{k}}$ is the superconductor gap, of the lead $\eta = L, R$. $\Psi_{\eta\vec{k}\sigma}^\dagger$ and $\Psi_{\eta\vec{k}\sigma}$ are the Nambu spinors

$$\Psi_{\eta\vec{k}\sigma}^\dagger = \begin{pmatrix} a_{\eta\vec{k}\sigma}^\dagger & a_{\eta,-\vec{k},-\sigma} \end{pmatrix}, \quad \Psi_{\eta\vec{k}\sigma} = \begin{pmatrix} a_{\eta\vec{k}\sigma} \\ a_{\eta,-\vec{k},-\sigma}^\dagger \end{pmatrix}.$$
$H_D$ is the Hamiltonian for the single-level quantum dot of energy $E_d$:

$$H_D = \sum_{\sigma} \phi_{\sigma}^d H^{QD} \phi_{\sigma}. \quad (5)$$

with

$$H^{QD} = \begin{pmatrix} E_d + U_d n_{-\sigma} & 0 \\ 0 & -E_d - U_d n_{\sigma} \end{pmatrix} \quad (6)$$

The tunneling Hamiltonian $H_T$ is given by

$$H_T = \sum_{\eta \vec{k} \sigma} \Psi_{\eta \vec{k} \sigma}^l H_{\eta \vec{k} \sigma}^l \phi_{\sigma}. \quad (7)$$

with

$$H_{\eta \vec{k}}^l = \begin{pmatrix} V_{\eta \vec{k}} & 0 \\ 0 & -V_{\eta \vec{k}} \end{pmatrix} \quad (8)$$

$H_T$ connects the dot to the biased superconducting leads and it allows the electric charge flow. $V_{\eta \vec{k}}$ is the hybridization matrix element between a conduction electron of energy $\varepsilon_{\eta \vec{k}}$ in the $\eta = L, R$ superconductor lead and a localized electron on the dot with energy $E_d$. $\phi_{\sigma}^d$ and $\phi_{\sigma}$ are the dot spinors

$$\phi_{\sigma}^d = \begin{pmatrix} d_{\sigma}^+ \\ d_{-\sigma}^- \end{pmatrix}, \quad \phi_{\sigma} = \begin{pmatrix} d_{\sigma}^- \\ d_{\sigma}^+ \end{pmatrix} \quad (9)$$

Here $a_{\eta \vec{k} \sigma}^d$ (or $a_{\eta \vec{k} \sigma}$) denotes the creation (annihilation) operator for a conduction electron with the wave vector $\vec{k}$, spin $\sigma$ in the $\eta = L, R$ superconductor lead. $d_{\sigma}^+(d_{\sigma})$ is the creation (annihilation) operator for an electron on the dot.

The flow of electric charge from the terminal $\eta$ is given by

$$I_\eta(t) = (-e) \frac{d}{dt} \langle N_\eta(t) \rangle = \frac{i e}{\hbar} [\langle HT(t), N_\eta(t) \rangle], \quad (10)$$

where $-e$ is the electron charge. $\langle \cdots \rangle$ is the thermodynamical average over the biased $L$ and $R$ leads at the temperature $T$. Equation (10) can be expressed in terms of the Keldysh Green function

$$F_{\eta \vec{k} \sigma}(t, t') \equiv -i \langle T_c a_{\eta \vec{k} \sigma}(t) d_{\sigma}^+(t') \rangle \quad (11)$$

as

$$I_\eta(t) = \frac{2 e}{\hbar} V_\eta \Re \sum_{\vec{k} \sigma} F_{\eta \vec{k} \sigma}^<(t, t), \quad (12)$$

where $F_{\eta \vec{k} \sigma}^<(t, t')$ is a lesser Keldysh Green function. For the purpose of the single particle current evaluation the coupling $|V_{\eta \vec{k}}|^2$ can be replaced by an average $V_\eta^2$ at the Fermi surfaces of the leads $L$ and $R$. Hereafter, for simplicity, we replace $V_{\eta \vec{k}}$ by $V_\eta$ as we already do it in eqn. (12).
The first evaluation step of $F_{\eta \vec{k} \sigma} \left( t, t' \right)$ expresses it in terms of dot Keldysh Green functions. Then, we set an equation of motion for the Keldysh Green function $F_{\eta \vec{k} \sigma} \left( t, t' \right)$

$$\left( i \frac{\partial}{\partial t} - \epsilon_{\eta \vec{k}} \right) F_{\eta \vec{k} \sigma} \left( t, t' \right) = -\sigma \Delta_{\eta} F_{\eta \vec{k} \sigma} \left( t, t' \right) + V_{\eta} G_{\sigma} \left( t, t' \right),$$  \hspace{1cm} (13)

where

$$F_{\eta \vec{k} \sigma} \left( t, t' \right) = -i \left\langle T_{c} a_{\eta \vec{k}, \sigma}^{\dagger} \left( t \right) d_{\sigma}^{\dagger} \left( t' \right) \right\rangle,$$ \hspace{1cm} (14)

and

$$G_{\sigma} \left( t, t' \right) = -i \left\langle T_{c} d_{\sigma} \left( t \right) d_{\sigma}^{\dagger} \left( t' \right) \right\rangle.$$ \hspace{1cm} (15)

Similarly, $F_{\eta \vec{k} \sigma} \left( t, t' \right)$ satisfies the equation of motion

$$\left( i \frac{\partial}{\partial t} + \epsilon_{\eta \vec{k}} \right) F_{\eta \vec{k} \sigma} \left( t, t' \right) = -\sigma \Delta_{\eta} F_{\eta \vec{k} \sigma} \left( t, t' \right) - V_{\eta} G_{\sigma} \left( t, t' \right),$$ \hspace{1cm} (16)

where

$$G_{\sigma} \left( t, t' \right) = -i \left\langle T_{c} d_{\sigma} \left( t \right) d_{\sigma}^{\dagger} \left( t' \right) \right\rangle.$$ \hspace{1cm} (17)

The eqns (13) and (16) can be written as follows:

$$\left( \frac{i}{\sigma} \frac{\partial}{\partial t} - \epsilon_{\eta \vec{k}} - \frac{\sigma \Delta_{\eta}}{i \frac{\partial}{\partial t} + \epsilon_{\eta \vec{k}}} \right) \left( \begin{array}{c} F_{\eta \vec{k} \sigma} \left( t, t' \right) \\ F_{\eta \vec{k} \sigma} \left( t', t \right) \end{array} \right) = \left( \begin{array}{cc} G_{\sigma} \left( t, t' \right) & V_{\eta} \sigma z \\ G_{\sigma} \left( t', t \right) & G_{\sigma} \left( t', t' \right) \end{array} \right) \times V_{\eta} \sigma z \\$$

$$\times \left( \begin{array}{c} \eta \vec{k} \sigma \left( t, t' \right) \\ \eta \vec{k} \sigma \left( t', t \right) \end{array} \right);$$ \hspace{1cm} (18)

This equation can be written as an integral along the Keldysh contour $C_{K}$

$$\left( \begin{array}{c} F_{\eta \vec{k} \sigma} \left( t, t' \right) \\ F_{\eta \vec{k} \sigma} \left( t', t \right) \end{array} \right) = \int_{C_{K}} dt'' \left( \begin{array}{c} \eta \vec{k} \sigma \left( t, t'' \right) \\ \eta \vec{k} \sigma \left( t', t'' \right) \end{array} \right) \times \left( \begin{array}{c} G_{\sigma} \left( t''', t'' \right) \\ G_{\sigma} \left( t'', t' \right) \end{array} \right),$$ \hspace{1cm} (19)

The $2 \times 2$ matrix in the right hand side of eqn (18) is an unperturbed Keldysh Green function where

$$\eta \vec{k} \sigma \left( t, t' \right) = -i \left\langle T_{c} a_{\eta \vec{k}, \sigma} \left( t \right) a_{\eta \vec{k}, \sigma}^{\dagger} \left( t' \right) \right\rangle_{0},$$ \hspace{1cm} (20)

$$\bar{\eta} \vec{k} \sigma \left( t, t' \right) = -i \left\langle T_{c} a_{\eta \vec{k}, \sigma}^{\dagger} \left( t \right) a_{\eta \vec{k}, \sigma} \left( t' \right) \right\rangle_{0},$$ \hspace{1cm} (21)

$$\bar{\eta} \vec{k} \sigma \left( t, t' \right) = -i \left\langle T_{c} a_{\eta \vec{k}, \sigma} \left( t \right) a_{\eta \vec{k}, \sigma} \left( t' \right) \right\rangle_{0},$$ \hspace{1cm} (22)

$$\bar{\eta} \vec{k} \sigma \left( t, t' \right) = -i \left\langle T_{c} a_{\eta \vec{k}, \sigma} \left( t \right) a_{\eta \vec{k}, \sigma} \left( t' \right) \right\rangle_{0}.$$ \hspace{1cm} (23)

The subindex $0$ indicates that evaluations are performed with $V_{\eta} = 0$.

The contribution $F_{\eta \vec{k} \sigma} \left( t, t' \right)_{SP}$ to the single particle (SP) current is given by
\[ \begin{align*}
\Gamma_{\eta} (t, t')_{SP} &= V_{\eta} \int_{-\infty}^{\infty} dt'' \times \\
& \left[ g^{(r)}_{\eta k} (t, t'') G_{\sigma}^> (t'', t') + g^{<}_{\eta k} (t, t'') G_{\sigma}^{(a)} (t'', t') \right] \quad (24)
\end{align*} \]

where we used eqn (19) and Langreth rules [22]. The superscripts <,>, (r), (a) correspond to lesser, greater, retarded and advanced Keldysh Green functions, respectively. Therefore, the single particle current \( I_{\eta} (t)_{SP} \) can be written as

\[ I_{\eta} (t)_{SP} = \frac{2e}{\hbar} \Re \sum_{\sigma} \int_{-\infty}^{\infty} dt' \left[ \Sigma^{(r)}_{\eta \sigma} (t, t') G_{\sigma}^< (t', t) + \Sigma^{<}_{\eta \sigma} (t, t') G_{\sigma}^{(a)} (t', t) \right] \quad (25) \]

\( \Sigma^{(r)}_{\eta \sigma} (t, t') = V_{\eta}^{2} \sum_{k} g^{(r)}_{\eta k} (t, t') \) and \( \Sigma^{<}_{\eta \sigma} (t, t') = V_{\eta}^{2} \sum_{k} g^{<}_{\eta k} (t, t') \) are self energies which are evaluated for isolated superconductors leads \( L \) \( R \). They depend on \( t \) and \( t' \) through \( t - t' \) and are independent of \( \sigma \). Their Fourier transforms are given by

\[ \begin{align*}
\Sigma^{(r)}_{\eta} (\omega) &= -\Gamma_{\eta} \left[ \frac{\omega - \mu_{\eta}}{\Delta_{\eta}} \zeta(\Delta_{\eta}, \omega - \mu_{\eta}) + i \zeta(\omega - \mu_{\eta}, \Delta_{\eta}) \right] \quad (26) \\
\Sigma^{<}_{\eta} (\omega) &= 2i \Gamma_{\eta} \zeta(\omega - \mu_{\eta}, \Delta_{\eta}) f(\omega - \mu_{\eta}) \quad (27)
\end{align*} \]

where

\[ \zeta (\omega, \omega') \equiv \Theta (|\omega| - |\omega'|) \frac{|\omega|}{\sqrt{\omega^2 - \omega'^2}} \quad (28) \]

\( \Gamma_{\eta} = \pi N_{\eta} (0) V_{\eta}^{2} \) are the coupling constants between the leads and the quantum dot in the wide band limit. \( N_{\eta} (0) \) is the density of states at the \( \eta \) Fermi level and \( f (\omega) \) is the Fermi-Dirac distribution function.

Equation (25) becomes

\[ I_{\eta} (t)_{SP} = \frac{2e}{\hbar} \Re \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i(\omega - \omega')t} \times \\
\left[ \Sigma^{(r)}_{\eta} (\omega) \sum_{\sigma} G_{\sigma}^> (\omega, \omega') + \Sigma^{<}_{\eta} (\omega) \sum_{\sigma} G_{\sigma}^{(a)} (\omega, \omega') \right] \quad (29) \]

Dot Keldysh Green's functions \( G_{\sigma}^> (\omega, \omega') \) and \( G_{\sigma}^{(a)} (\omega, \omega') \) are straightforward evaluated. It turns out that they are \( \sigma \) independent and frequency diagonal in the stationary limit

\[ \begin{align*}
G_{\sigma}^> (\omega, \omega') &\equiv 2\pi \delta (\omega - \omega') G^< (\omega) \quad (30) \\
G_{\sigma}^{(a)} (\omega, \omega') &\equiv 2\pi \delta (\omega - \omega') G^{(a)} (\omega), \quad (31)
\end{align*} \]

Equation (29) becomes

\[ I_{\eta \sigma} = \frac{4e}{\hbar} \Re \int_{-\infty}^{\infty} d\omega \left[ \Sigma^{(r)}_{\eta} (\omega) G^< (\omega) + \Sigma^{<}_{\eta} (\omega) G^{(a)} (\omega) \right] \quad (32) \]
The final expression for the single particle current $I_{SP} \equiv (I_{R,SP} - I_{L,SP})/2$ is given by

$$I_{SP} = \frac{8\pi e}{h} \int_{-\infty}^{\infty} d\omega \frac{\Gamma_L(\omega - eV)}{\Gamma_L(\omega - eV) + \Gamma_R(\omega)} \rho(\omega) \left[ f(\omega - eV) - f(\omega) \right],$$

(33)

In eqn (33) we performed a trivial shift of the dot energy level and insert the electric potential $V$ through $eV = \mu_L - \mu_R$. The extra $2\pi$ factor arises from the dot Keldysh Green functions. $\Gamma_\eta(\omega)$ and $\rho(\omega)$ are given by

$$\Gamma_\eta(\omega) = \Gamma_\eta\zeta(\omega, \Delta_\eta)$$

(34)

$$\rho(\omega) = -\frac{1}{\pi} \Im G^{(r)}(\omega) = \frac{\Gamma(\omega)/\pi}{(\omega - E_d)^2 + \Gamma^2(\omega)}$$

(35)

Here $\rho(\omega)$ is the so-called quantum dot spectral function which is given in terms of the retarded $G^{(r)}(\omega)$ Keldysh Green function [18]. At steady state there is no net flow 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

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

(36)

which becomes a weighted average over the $L$ and $R$ contacts

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

(37)

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, drain and gate applied voltages. Since the number of quantum levels in the channel is small the particle number variation is negligible. It amounts to neglect potential profile variation inside the channel. Then we can visualize the channel as a single point and an equivalent circuit framework is quite useful. In this framework we associate capacitances $C_D$, $C_S$ y $C_G$ to the drain, source and gate, respectively. Whenever drain, source and gate bias potentials $V_D$, $V_S$ and $V_G$, respectively, are present it induces a shift $U = -e(V_{ch} - V_0)$ of the electrostatic energy inside the channel. $V_{ch}$ and $V_0$ are channel electrostatic potentials after and before we apply the source and drain biases, respectively. The electronic population before and after we apply the biases mentioned above are given by

$$-eN_0 = C_D V_0 + C_S V_0 + C_G V_0$$

$$-eN = C_D (V_{ch} - V_D) + C_S (V_{ch} - V_S) + C_G (V_{ch} - V_G),$$

(38)

(39)

respectively. It leads us to

$$-e\Delta N = -e(N - N_0) = C_E (V_{ch} - V_0) - C_D V_D - C_S V_S - C_G V_G$$

(40)
where $C_E = C_D + C_S + C_G$. The electrostatic potential shift $U$ inside the channel becomes

$$U = U_L + \frac{e^2}{C_E} \Delta N$$

(41)

where

$$C_E U_L \equiv C_D (-eV_D) + C_S (-eV_S) + C_G (-eV_G)$$

(42)

The first term yields linear contributions to the potential profile while the second one introduces a direct dependence on the electronic population $N$. $U_0 = e^2/C_E$ 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.

The potential profile $U$ shifts the dot quantum levels such that $I_{SP}$ and $N$ are found from a system of self consistent equations.

$$I_{SP} = \frac{8\pi e}{h} \int_{-\infty}^{\infty} d\omega \frac{\Gamma_L (\omega - eV) \Gamma_R (\omega)}{\Gamma_L (\omega - eV) + \Gamma_R (\omega)} \rho (\omega - U) [f (\omega - eV) - f (\omega)] ,$$

(43)

$$N = 2 \int_{-\infty}^{\infty} d\omega \rho (\omega - U) \frac{\Gamma_L (\omega - eV) f (\omega - eV) + \Gamma_R (\omega) f (\omega)}{\Gamma_L (\omega - eV) + \Gamma_R (\omega)} .$$

(44)

Equation (44) determines $N$ in a self consistent fashion which immediately yields the single particle electric current $I_{SP}$ by carrying out the integration in eqn (43).

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 and Discussion

In the dashed curve in Figure 1 we show zero temperature $I-V$ characteristics, calculated without the self consistent field (non-SFC) method for values of gate voltage $V_g > 0$. In the same figure the solid curve shows zero temperature $I-V$ characteristics, calculated with the self consistent field (SCF) method for values of gate voltage $V_g > 0$. As we can see in the dashed curve, the current is nonzero for positive values of the drain voltage, while for negative values of the drain voltage the current vanishes out. For the solid curve the current can have nonzero values.

In Figure 2 we show zero temperature $I-V$ characteristics for gate voltage values $V_g < 0$ which are calculated without the self consistent (non-SCF) method (dashed curve) and with the self consistent method (SCF) (solid curve). In the first case (non-SCF) the current is zero for positive values of the drain voltage and nonzero for negative values of the drain voltage, while in the second case (SCF) we can observe a symmetric $I-V$ characteristic.
Figure 1: Zero temperature I-V characteristics calculated without the self consistent field (non-SCF) method (dashed curve) and calculated using the self consistent field (SCF) method (solid curve), with $E_d = 0.2$ 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 self consistent field (non-SCF) method (dashed curve) and calculated using the self consistent field (SCF) method (solid curve), with $E_d = 0.2$ 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.
On the other hand, when we use the self consistent field (SCF) method, the single particle current reaches the maximum value for higher drain voltage as compared to the non-SCF method. It means that the presence of the potential profile $U$ inhibits the electron flow. Furthermore, it is noted that the $I – V$ characteristics, as calculated with the self consistent field (SCF) method, agree with experimental data reported in the literature [23]. In addition, it proves that the single particle electric current can have nonzero values for positive and negative values of the drain voltage.

4. Conclusions

In conclusion, we have studied the effect of a self consistent potential profile on single particle electric current across a mesoscopic system attached to superconductor leads. Such system describes a spin degenerated single quantum where Coulomb blockade is neglected, in the regime $\Delta \gg \Gamma_{L,R}$. We derived an exact single particle electric current by means of the many body Keldysh technique. Zero temperature $I – V$ characteristics agree with the experimental results. Furthermore, we showed there are symmetric $I – V$ characteristic, within the self consistent method which address an interplay among potential profile, single particle electric current and electronic population at the mesoscopic region.

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