Self-consistent current-voltage characteristics of superconducting nano-structures.

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Abstract

By solving the Bogoliubov - de Gennes equation self-consistently in the presence of a non-equilibrium quasi-particle distribution, we compute the current-voltage characteristic of a phase coherent superconducting island with a tunnel barrier at one end. The results show significant structure, arising from the competition between scattering processes at the boundaries of the island and modification of the order parameter by quasi-particles and superflow. This structure is not present in non self-consistent descriptions of normal-superconducting nano-structures.

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It is now well established that coherent Andreev scattering provides the key to understanding transport in mesoscopic superconductors and normal-superconducting (N-S) interfaces. For example, zero bias anomalies[1] can be understood through a description based on multiple Andreev scattering in N-S tunnel junctions[2-5], while phase periodic conductances in N-S-N nano-structures[6] are understandable through theories of coherent transport which neglect inelastic scattering[7-14]. All of the above theoretical descriptions are based on non-self-consistent solutions of the Bogoliubov de-Gennes equation or corresponding quasi-classical equations and are not capable of describing the modification of a superconducting order parameter by a transport current. Effects of this kind are observable as super-gap structure in the differential conductance of N-S tunnel junctions and point contacts[15,16], but to date, there exists no quantitative theoretical framework for their understanding. For structures smaller than the inelastic phase breaking length $l_\phi$, such features cannot be ascribed to quasi-particle “heating”, because the energy of the electron is preserved during its passage through the sample. Instead, any modification is a hot electron effect and requires a description which takes into account the non-equilibrium distribution of electrons within the sample.

A theoretical description which encompasses both non-equilibrium effects of this kind and phenomena associated with phase coherent transport does not currently exist. The aim of this Paper is to provide the first self-consistent description of phase coherent transport in a N-S-N structure, based on exact solution of the BdG equation. Motivated by the success of the Blonder, Tinkham and Klapwijk[17] (BTK) calculation for the current-voltage (I-V) characteristic of a N-S interface with a delta function scatterer, we examine the simplest possible generalisation which is capable of highlighting the new physics which emerges from a self-consistent description. The system of interest is
a mesoscopic scattering region containing a superconducting island connected to perfect normal leads, which are in turn connected to external reservoirs at chemical potentials $\mu_1$ and $\mu_2$. The system length $L$ is assumed to be smaller than a quasi-particle phase breaking length and therefore a description, which incorporates quasi-particle phase coherence throughout the system is appropriate. The main question of interest is whether or not such a description yields observable super-gap structure, which is absent from a BTK description, thereby obviating the need to introduce ad hoc heating effects.

Before discussing quantitative results, it is useful to identify characteristic voltages which are missing from the BTK description[17]. For convenience, consider the zero temperature limit and choose $\mu_1 \geq \mu_2$. In this case electrons (holes) are incident on the island from the left (right) reservoir over an energy interval $0 < E < \mu_1 - \mu$ ($0 < E < \mu - \mu_2$), where $\mu$ is the self-consistently determined condensate chemical potential. The associated current will both suppress the magnitude of the order parameter and generate a phase gradient. For a homogeneous superconductor with an order parameter $\Delta(x) = \Delta_0 \exp[iv_s x]$, the energy gap for excitations parallel (anti-parallel) to the phase gradient $v_s$ is $\mu_- = \Delta_0 - p_F v_s$ ($\mu_+ = \Delta_0 + p_F v_s$), where $p_F$ is the Fermi momentum. For a long enough island, where the order parameter at the centre of the island is approximated by the above form, excitations incident on the superconductor with energies less than these values will be reflected and therefore in addition to the voltage $\Delta_0/e$, one might naively expect the I-V characteristic to show some feature when the reservoir potentials satisfy $\mu_1 - \mu = \mu_\pm$ or $\mu - \mu_2 = \mu_\pm$. In addition one might expect features to occur for those values of $\mu_1 - \mu_2$ at which $\Delta_0 - p_F v_s = 0$ and at which the self-consistent value of $\Delta(x)$ vanishes everywhere.

To obtain a self-consistent description, we solve the Bogoliubov - de Gennes
equation

\[ H(x) \begin{pmatrix} u_n(x) \\ v_n(x) \end{pmatrix} = E_n \begin{pmatrix} u_n(x) \\ v_n(x) \end{pmatrix} \]  

(1)

with a Hamiltonian

\[ H(x) = \begin{pmatrix} \left[-(\hbar^2/2m)\partial_x^2 + u(x) - \mu\right] & \Delta(x) \\ \Delta^*(x) & \left[-(\hbar^2/2m)\partial_x^2 + u(x) - \mu\right] \end{pmatrix} \]  

(2)

where \( \mu \) is the condensate chemical potential, \( u(x) \) is the normal scattering potential and \( \Delta(x) \) the superconducting order parameter, defined self-consistently by the following equation

\[ \Delta(x) = V(x) \left( \sum_{E_n>0} ' u_n^*(x)v_n(x) - \sum_{E_n>0} ' u_n^*(x)v_n(x)\langle\langle \gamma_{n\sigma}^\dagger(x)\gamma_{n\sigma}(x)\rangle\rangle \right) \]  

(3)

In this expression, primes on the sums indicate that only terms with \( E_n \) less than some cut-off \( E_c \) are to be included, due to the fact that the electron-electron interaction is only attractive over a small range of energies near the Fermi surface, \( \gamma_{n\sigma}^\dagger \) creates a Bogoliubov quasi-particle and double angular brackets indicate a trace over the density matrix of the system. In what follows, the pairing potential \( V(x) \) is chosen to equal a constant for \( 0 < x < L \) and to vanish outside this interval. The normal scattering potential is chosen to be \( u(x)/\mu_0 = (2Z/k_F)\delta(x) \), where \( \mu_0 \) is the condensate chemical potential in the absence of an applied voltage and \( k_F = (2m\mu_0/\hbar^2)^{1/2} \). For a given choice of \( L, Z, E_c, V_0 \) and reservoir potentials, both the magnitude and phase of \( \Delta(x) \) will be computed at all points in space, along with the condensate chemical potential \( \mu \).

Since we are interested in an open system, equation (3) involves sums over all incoming scattering states, integrated over all \( E < E_c \). At zero temperature, for the case \( \mu_1 > \mu > \mu_2 \), quasi-particle states corresponding to incoming electrons (holes)
are incident from reservoir 1 (2) over energy intervals $\mu_1 - \mu$ ($\mu - \mu_2$). Assuming these intervals are less than the cut-off $E_c$ and if a scattering state of energy $E$ corresponding to an incident quasi-particle of type $\alpha$ from reservoir $i$ has a particle (hole) amplitude $u_{i\alpha}(x, E)$ ($v_{i\alpha}(x, E)$), then equation (3) reduces to

$$
\Delta(x) = V(x) \sum_{i=1}^{2} \frac{1}{2} \int_{0}^{E_c} ((u_{i-}^*(x, E)u_{i-}(x, E)) + ((u_{i+}^*(x, E)v_{i+}(x, E)))dE
$$

$$
- V(x) \int_{0}^{\mu_1 - \mu} (u_{1+}^*(x, E)v_{1+}(x, E))dE
$$

$$
- V(x) \int_{0}^{\mu - \mu_2} (u_{2-}^*(x, E)v_{2-}(x, E))dE
$$

(4)

To calculate scattering solutions in the region occupied by the island, we start from an initial guess for $\Delta(x)$ and $\mu$ and divide the interval $0 < x < L$ into a large number of small cells of size $<< k_F^{-1}$, within which $\Delta(x)$ and $u(x)$ are assumed constant. If $T(x_0)$ is the matrix obtained by producting together transfer matrices associated with all cells in the interval $0 < x < x_0$ and then as outlined in appendix 1 of reference[18], the scattering matrix $S$ of the island can be obtained from the transfer matrix $T(L)$. Within the external leads, the most general eigenstate of $H$ belonging to eigen-energy $E$ is a linear superposition of plane waves. For a given incoming plane wave, a knowledge of $S$ yields the plane wave amplitudes on the left side of the island, which can be combined with $T(x_0)$ to yield the wavefunction at $x = x_0$. Given these solutions, $\Delta(x)$ is re-evaluated using equation (4) and a new choice for $\mu$ is obtained by insisting that the currents $j_1$ and $j_2$ in the leads attached to reservoirs 1 and 2 are equal. This process is repeated until the root mean square difference between successive order parameters is less than 1% of the magnitude of $\Delta(L/2)$. 
In what follows all results are for an island of length $L k_F = 750$, a cut-off of $E_c = 0.085\mu_0$ and a pairing potential of magnitude $V = 0.28\mu_0$. For an infinite homogeneous superconductor with no current flowing and a density of states $n(0)$, BCS theory predicts a bulk order parameter of magnitude $\Delta_0 = E_c / \sinh\left\{1/[n(0)V]\right\}$, which for this choice of parameters yields $\Delta_0 \approx 0.005\mu_0$. As an example of the results obtained, for an island with no barrier (ie $Z = 0$), figure 1 shows self-consistent results for the magnitude $|\Delta(x)|$ and phase $\phi(x)$ of the order parameter, for various applied reservoirs potential differences. As expected, $|\Delta(x)|$ reaches a maximum value at $x = L/2$ and is suppressed at the ends of the island, on a length scale $\xi = k_F^{-1}\mu/|\Delta(L/2)|$, whereas the corresponding phase gradient $v_s(x) = \nabla\phi(x)$ is almost a constant. Furthermore the zero voltage value of $\Delta(L/2)$, (denoted $\Delta_0$ in what follows) agrees with the BCS prediction.

In what follows, we denote $v_s(L/2)$ and $|\Delta(L/2)|$ by $v_s$ and $\Delta_s$ respectively.

By repeating these calculations for a range of reservoir potentials and barrier strengths, one obtains I-V curves, whose derivative yields the differential conductance shown in figure 2. Clearly these curves exhibit structure which is not present in a non self-consistent description[17]. To identify the underlying physical processes, figure 3 shows self-consistently determined values of $\Delta_s$ and the various characteristic voltages identified above, plotted against the reservoir potential difference. For each value of $Z$, the upper and lower dashed lines of figure 3 show results for $\mu_+$ and $\mu_-$ respectively, while the thin solid line shows $\Delta_s$. The upper and lower thick solid lines show values of $\mu_1 - \mu$ and $\mu - \mu_2$ respectively. For $Z = 0$, where $\mu = (\mu_1 - \mu_2)/2$, the latter are equal. More generally, for the range of voltages studied, one finds $\mu = \mu_2 + \alpha(\mu_1 - \mu_2)$, where $\alpha = 0.5, 0.421, 0.241, 0.126$ for $Z = 0, 0.25, 0.55, 0.83$, respectively. Maxima and minima in the differential conductance of figure 2 are associated with various crossings in figure 3.
Consider for example the $Z = 0.55$ and $Z = 0.83$ results, where the first maximum in $G_N^{-1} \partial I/\partial (\mu_1 - \mu_2)$ corresponds to the crossing $\mu_1 - \mu = \Delta_s$. For these structures, provided $\mu - \mu_2 < \mu_-$, excitations from the right reservoir (2) are almost completely Andreev reflected at $x = L$ and therefore the conductance is dominated by scattering of electrons from the left reservoir at $x = 0$. In this limit, it is of interest to examine the quantity $G_N^{-1} \partial I/\partial (\mu_1 - \mu)$, which in the absence of quasi-particle transmission, is equivalent to the left boundary conductance, examined by BTK. The solid lines of figure 4 show self-consistent results for this quantity. For comparison, the dashed lines show non self-consistent results (which are essentially those of BTK[17]) obtained by insisting that $\mu = \mu_2$ and for $0 < x < L$, $\Delta(x) = \Delta_0$. For $Z = 0.83$ the dashed and solid curves of figure 4 are in good agreement, reflecting the fact that for large $Z$ the current is small and therefore $\Delta(x)$ is not significantly modified. For the smaller barrier strength, the self-consistent conductance differs significantly from the BTK curve. In the presence of quasi-particle transmission [18,20], the resistance of a N-S-N structure does not reduce to the sum of two boundary resistances. Consequently even for $Z = 0.83$, the N-S-N differential conductance of figure 2 shows extra structure which is absent from a boundary conductance calculation. For example the second peak of the $Z = 0.83$ results of figure 2 corresponds to the crossing $\mu - \mu_2 = \Delta_s - v_s p_F$, while the minimum between these peaks corresponds to the crossing $\mu_1 - \mu = \Delta_s + v_s p_F$. For $Z = 0.55$ the peaks at $\mu_1 - \mu$ and $\mu - \mu_2$ are no longer separated, but again a minimum occurs at $\mu_1 - \mu = \Delta_s + v_s p_F$. For this value of $Z$, a maximum occurs at $\mu_1 - \mu_2 \sim 3\Delta_s$, at which the magnitude of $\Delta(L/2)$ starts to become significantly reduced by the current.

To obtain the above results, we have presented the first self-consistent description of a superconducting nano-structure, which incorporates quasi-particle phase coherence and non-equilibrium effects. The computed current-voltage characteristic of a single superconducting island is the result of several competing phenomena associated
with quasi-particle scattering from boundaries and modification of the order parameter by both superflow and a non-equilibrium quasi-particle distribution. This competition produces significant new structure, particularly at energies above $\Delta_0$, which is not contained within a non self-consistent description. This structure is observable experimentally [19] but in earlier discussions[15] has been dismissed as a distortion due to heating.

**Note added in proof**

A similar calculation has been carried out recently by F.Sols and J. Sanchez-Canizarez, in which the superconductor is treated as an incoherent reservoir[21]. Where agreement is expected, their results are comparable with those reported here.

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Figure captions

Figure 1. Results for the case $Z = 0$. The upper figure shows the form of the attractive interaction $V(x)$ (in units of $\mu_0$) used in all the calculations of this paper. The middle and lower graphs show the self-consistent forms the magnitude and phase of $\Delta(x) = |\Delta(x)| \exp i\phi(x)$. The results with the largest values of $|\Delta(x)|$ and constant phase correspond to $\mu_1 - \mu_2 = 0$. In order of decreasing $|\Delta(x)|$ and increasing phase gradient, remaining results correspond to $\mu_1 - \mu_2 = 0.006$ and $\mu_1 - \mu_2 = 0.01$, respectively.

Figure 2. Self-consistent results for the differential conductance of a superconducting dots, with a delta function barrier of strength $Z$, located at $x = 0$.

Figure 3. For each value of $Z$, the upper (lower) dashed line shows self-consistent results for the voltages $\mu_+ = \Delta_s + p_F v_s (\mu_- = \Delta_s - p_F v_s)$, while the thin solid line shows $\Delta_s = |\Delta(L/2)|$. The upper (lower) thick solid line shows self-consistent values of $\mu_1 - \mu (\mu - \mu_2)$. For $Z = 0$, the latter are equal.

Figure 4. The solid lines show self-consistent results for $G_N^{-1} \partial I / \partial (\mu_1 - \mu)$. The dashed lines show non self-consistent results obtained by setting $\Delta(x) = \Delta_s$ for $0 < x < L$ and zero elsewhere.