Self-consistent current-voltage characteristics of superconducting nanostructures

A. Martin and C. J. Lambert

School of Physics and Materials, Lancaster University, Lancaster LA1 4YB, England

(Received 19 December 1994)

By solving the Bogoliubov–de Gennes equation self-consistently in the presence of a nonequilibrium quasiparticle 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 quasiparticles and superflow. This structure is not present in non-self-consistent descriptions of normal-superconducting nanostructures.

It is now well established that coherent Andreev scattering provides the key to understanding transport in mesoscopic superconductors and normal-superconducting (NS) interfaces. For example, zero-bias anomalies can be understood through a description based on multiple Andreev scattering in NS tunnel junctions, while phase periodicty conductances in normal-superconducting-normal (NSN) nanostructures are understandable through theories of coherent transport which neglect inelastic scattering. All of the above theoretical descriptions are based on non-self-consistent solutions of the Bogoliubov–de Gennes (BdG) equation or corresponding quasiclassical 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 supergap structure in the differential conductance of NS tunnel junctions and point contacts, 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 quasiparticle 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 nonequilibrium distribution of electrons within the sample.

A theoretical description which encompasses both nonequilibrium effects of this kind and phenomena associated with phase-coherent transport does not currently exist. The aim of this paper is to provide a self-consistent description of phase-coherent transport in a NSN structure, based on exact solution of the BdG equation. Motivated by the success of the Blonder, Tinkham, and Klapwijk (BTK) calculation for the current-voltage ($I$-$V$) characteristic of a NS interface with a $\delta$-function scatterer, we examine the simplest possible generalization, 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 the quasiparticle phase-breaking length and therefore a description which incorporates quasiparticle phase coherence throughout the system is appropriate. The main question of interest is whether or not such a description yields observable supergap 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. 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 $\Delta(x) = \Delta_0 \exp[i \phi(x)]$, the energy gap for excitations parallel (antiparallel) to the phase gradient $\nu_s(x)$ is $\mu_+ = \Delta_0 - \nu_s(x)$ ($\mu_- = \Delta_0 + \nu_s(x)$), where $\nu_s$ is the Fermi momentum. For a long enough island, where the order parameter at the center 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 $\mu_2 - \mu = \mu_\pm$. In addition, one might expect features to occur for those values of $\mu_1 - \mu_2$ at which $\Delta_0 - \nu_F \nu_s = 0$, 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

$$H(x) \begin{bmatrix} u_n(x) \\ v_n(x) \end{bmatrix} = E_n \begin{bmatrix} u_n(x) \\ v_n(x) \end{bmatrix},$$

with a Hamiltonian

$$H(x) = \begin{bmatrix} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + u(x) - \mu \right] & \Delta(x) \\ \Delta^*(x) & \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + u(x) - \mu \right] \end{bmatrix},$$
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:

$$
\Delta(x) = V(x) \left[ \sum' E_n > 0 u_n^*(x) v_n(x) - \sum' E_{\sigma} > 0 u_\sigma^*(x) v_\sigma(x) \right] \left( \langle \gamma_{\alpha \sigma}^+(x) \gamma_{\alpha \sigma}^-(x) \rangle \right) \right] \right]
$$

(3)

In this expression, primes on the sums indicate that only terms with $E_n$ less than some cutoff $E_c$ 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, $\gamma_{\alpha \sigma}$ creates a Bogoliubov quasiparticle, 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, Eq. (3) involves sums over all incoming scattering states, integrated over all $E < E_c$. At zero temperature, for the case $\mu_1 > \mu > \mu_2$, quasiparticle 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 cutoff $E_c$, and if a scattering state of energy $E$ corresponding to an incident quasiparticle of type $\alpha$ from reservoir $i$ has a particle (hole) amplitude $u_{i\alpha}(x,E)$ [$v_{i\alpha}(x,E)$], then Eq. (3) reduces to

$$
\Delta(x) = V(x) \sum_{i=1}^2 \frac{1}{2} \int_0^{E_c} \left[ [u_{i+}(x,E) v_{i-}(x,E)] 
$$

$$
+ [u_{i-}^*(x,E) v_{i+}^*(x,E)] \right] dE
$$

$$
- V(x) \int_0^{\mu_1 - \mu} [u_{i+}^*(x,E) v_{i+}(x,E)] dE
$$

$$
- V(x) \int_0^{\mu - \mu_2} [u_{i-}^*(x,E) v_{i-}(x,E)] dE \right].
$$

(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 producing together transfer matrices associated with all cells in the interval $0 < x < x_0$ and then as outlined in Appendix 1 of Ref. 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 eigenenergy $E$ 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 wave function at $x = x_0$. Given these solutions, $\Delta(x)$ is reevaluated using Eq. (4) and a new value for $\mu$ is obtained by insisting that the currents $I_1$ and $I_2$ in the leads attached to reservoirs 1 and 2 are equal. This process yields the magnitude of $\Delta(x)$ and phase of $\Delta(x)$ at each point in space and in what follows, and 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 cutoff 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 $\Delta_0 = E_c / \sinh[1/(n(0)V)]$, 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 (i.e., $Z = 0$), Fig. 1 shows self-consistent results for the magnitude $|\Delta(x)|$ and phase $\phi(x)$ of the order parameter, for various applied reservoir 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 $\phi(x)$ 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 $v_3(L/2)$ and $|\Delta(L/2)|$ by $v_3$ and $\Delta_3$, 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 Fig. 2. Clearly these curves exhibit structure...
FIG. 2. Self-consistent results for the differential conductance of a superconducting dot, with a δ-function barrier of strength $Z$, located at $x = 0$.

which is not present in a non-self-consistent description. To identify the underlying physical processes, Fig. 3 shows self-consistently determined values of $\Delta$, 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 Fig. 3 show results for $\mu_+$ and $\mu_-$, respectively, while the thin solid line shows $\Delta_x$. The upper and lower thick solid line 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, and 0.126 for $Z = 0$, 0.25, 0.55, and 0.83, respectively. Maxima and minima in the differential conductance of Fig. 2 are associated with various crossings in Fig. 3.

Consider for example the $Z = 0.55$ and 0.83 results, where the first maximum in $G_N^{-1}[dI/d(\mu_1 - \mu_2)]$ corresponds to the crossing $\mu_1 - \mu = \Delta_x$. 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

FIG. 4. The solid lines show self-consistent results for $G_N^{-1}[dI/d(\mu_1 - \mu)]$, which, in the absence of quasiparticle transmission, is equivalent to the left boundary conductance examined by BTK. The solid lines of Fig. 4 show self-consistent results for this quantity. For comparison, the dashed lines show non-self-consistent results [which are essentially those of BTK (Ref. 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 Fig. 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 quasiparticle transmission, the resistance of a NSN structure does not reduce to the sum of two boundary resistances. Consequently even for $Z = 0.83$, the NSN differential conductance of Fig. 2 shows extra structure which is absent from a boundary conductance calculation. For example, the second peak of the $Z = 0.83$ results of Fig. 2 corresponds to the crossing $\mu - \mu_2 = \Delta_x - \nu_p$, while the minimum between these peaks corresponds to the crossing $\mu_1 - \mu = \Delta_x + \nu_p$. For $Z = 0.55$ the peaks at $\mu_1 - \mu$ and $\mu - \mu_2$ are no longer separated, but again a minimum occurs at $\mu_1 - \mu = \Delta_x + \nu_p$. For this value of $Z$, a maximum occurs at $\mu_1 - \mu \sim 3\Delta_0$, at which the magnitude of $\Delta(L/2)$ starts to become significantly reduced by the current.

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

Note added in proof. A similar calculation to the one
reported here has been carried out recently by Sols and Sanchez-Cañizares (Ref. 21), in which the superconductor is treated as an incoherent reservoir. Where agreement is expected, the results are comparable.

This work was supported in part from EEC via an HCM grant, by EPSRC, NATO, and the Institute for Scientific Interchange. We thank F. Sols, J. Sanchez-Cañizares, and V. C. Hui for interesting discussions.

19See, for example, Fig. 7 of Ref. 15 and Fig. 1 of Ref. 16.