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1996 J. Phys.: Condens. Matter 8 L731

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LETTER TO THE EDITOR

## Non-linear transport properties of superconducting nanostructures

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Received 2 July 1996, in final form 1 October 1996

**Abstract.** By solving the Bogoliubov–de Gennes equation self-consistently, we compute transport properties of a one dimensional superconducting island with a delta-function normal scatterer at the centre. The calculated  $I$ – $V$  characteristics 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. At a certain critical current, the order parameter exhibits a quasi-first-order transition to the normal state, smeared by the finite system size. At this point, the differential conductance is negative and can have a magnitude greater than  $2e^2/h$ , despite the fact that there is only a single scattering channel.

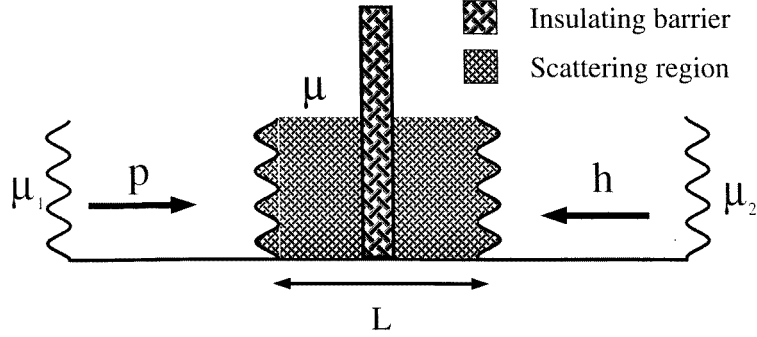
It is well established that phase-coherent Andreev scattering provides the key to understanding transport in mesoscopic normal–superconducting hybrid structures and that quantitative descriptions can be obtained using either quasi-classical or multiple-scattering methods [1–11].

In the absence of superconductivity, if a current  $I$  flows between two normal reservoirs at a potential difference  $V$ , then the differential conductance  $G = \partial I / \partial V$  is given by the Landauer formula  $G = (2e^2/h)T_0$ , which predicts that the conductance per channel possesses an upper bound of  $2e^2/h$ . In the linear-response limit, the multi-channel scattering theory proposed in [12] and [13] predicts that the upper bound persists, even in the presence of superconductivity, whereas the conductance per channel between a normal (N) and a superconducting (S) reservoir possesses an upper bound of  $4e^2/h$ . The aim of this letter is to provide a self-consistent description of phase coherent transport in such structures, which shows that beyond the linear-response region, when the order parameter is modified by the current, these bounds can be grossly violated.

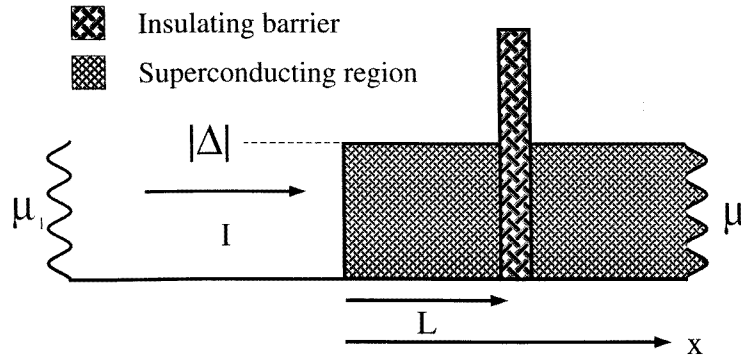
Figure 1 shows an N–S–I–S–N structure, formed when two normal (N) reservoirs of chemical potentials  $\mu_1$  and  $\mu_2$ , are attached to a scattering region comprising two superconducting regions (S) connected to an insulating region. Figure 2 shows a corresponding N–S–I–S structure, formed when normal and superconducting reservoirs connect to an S–I–S scattering region. In each case the superconductors possess a common spatially independent condensate chemical potential  $\mu$ . 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 significant structure which one would not obtain by performing a non-self-consistent calculation.

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

$$\begin{pmatrix} \mathcal{H}(x) & \Delta(x) \\ \Delta^*(x) & -\mathcal{H}^*(x) \end{pmatrix} \begin{pmatrix} u_n(x) \\ v_n(x) \end{pmatrix} = E_n \begin{pmatrix} u_n(x) \\ v_n(x) \end{pmatrix} \quad (1)$$



**Figure 1.** This diagram schematically shows the N-S-I-S structure, where quasi-particles impinge upon the scattering region from the left reservoir over an energy range  $\mu_1 - \mu$  and quasi-holes impinge upon the scattering region from the right reservoir over an energy range  $\mu - \mu_2$ .



**Figure 2.** This diagram schematically shows the N-S-I-S structure.

with

$$\mathcal{H}(x) = -\frac{\hbar}{2m} \partial_x^2 + U_0(x) - \mu \quad (2)$$

where  $\mu$  is the condensate chemical potential,  $U_0(x)$  is the normal potential and  $\Delta(x) = |\Delta(x)|e^{i\theta(x)}$  the superconducting order parameter, given by

$$\Delta(x) = V(x) \sum_{\substack{n>0 \\ \sigma}} (v_n(x) u_n^*(x)) \left( \frac{1}{2} - \langle \gamma_{n\sigma}^\dagger \gamma_{n\sigma} \rangle \right). \quad (3)$$

In this expression, the sum is over energies  $E_n$  less than a cut-off  $E_c$  due to the fact that the electron–electron interaction ( $V$ ) is only attractive over a 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. Since we solve the Bogoliubov–de Gennes equation in the presence of external leads, the trace is over scattering states of the open system.

In what follows the pairing potential  $V(x)$  is chosen to be equal to a constant for  $0 < x < L$  and to vanish outside this interval. The normal scattering potential is chosen to be  $u(x)/\mu = (2Z/k_F)\delta(x - L/2)$ , where  $\mu$  is the condensate chemical potential in the absence of an applied voltage and we define  $k_F = (2m\mu/\hbar^2)^{1/2}$ . 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, the above equation involves sums over all left- and right-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 the above equation reduces to

$$\begin{aligned} \Delta(x) = V(x) \sum_{i=1}^2 \frac{1}{2} \int_0^{E_c} & ((u_{i-}^*(x, E)v_{i-}(x, E)) + (u_{i+}^*(x, E)v_{i+}(x, E))) dE \\ & - V(x) \int_0^{\mu_1 - \mu} (u_{1+}^*(x, E)v_{1+}(x, E)) dE \\ & - V(x) \int_0^{\mu - \mu_2} (u_{2-}^*(x, E)v_{2-}(x, E)) dE. \end{aligned} \quad (4)$$

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 much less than  $k_F^{-1}$ , within which  $\Delta(x)$  and  $u(x)$  are assumed constant. If  $T(x_0)$  is the matrix obtained by multiplying together transfer matrices associated with all cells in the interval  $0 < x < x_0$  and then as outlined in appendix 1 of [13], 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-hand side of the island, which can be combined with  $T(x)$  to yield the wavefunction at all points  $x$ . Given these solutions,  $\Delta(x)$  is re-evaluated using the above equation 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  $\Delta(L/2)$ .

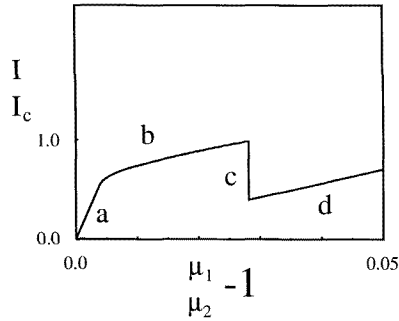
Before proceeding with a fully self-consistent calculation it is useful to examine a simpler problem, which is not fully self-consistent, but captures much of the physics contained in an exact solution [14]. To this end, consider the N-S-I-S structure of figure 2, which consists of a normal lead attached to a clean superconducting lead with a single normal scattering potential placed deep inside the superconductor at a position  $L \gg \xi$ . To obtain insight into the fully self-consistent problem, we first implement a quasi-self-consistent scheme in which  $\Delta(x) = |\Delta|$  for  $x > 0$  and  $\Delta(x) = 0$  for  $x < 0$ . The current  $I$  and the order parameter  $|\Delta|$  are then obtained by solving the following equations:

$$I = N(0)v_F \int_0^{\mu_1 - \mu} (1 - R_0 + R_a) dE \quad (5)$$

where  $R_0$  is the probability of normal reflection and  $R_a$  is the probability of Andreev reflection and

$$\frac{I}{I_c} = \left( \frac{4}{3\sqrt{3}} \right) \left( \frac{|\Delta|}{|\Delta_0|} \right)^2 \left( \sqrt{1 - \left( \frac{|\Delta|}{|\Delta_0|} \right)^2} \right) \quad (6)$$

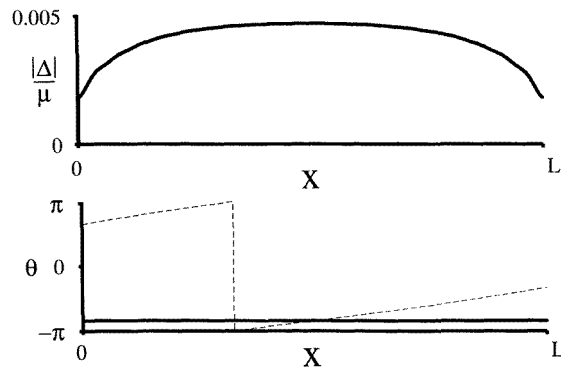
where  $I_c$  is the critical current of the superconducting lead and  $|\Delta_0|$  is the value of  $|\Delta|$  when  $I = 0$ .



**Figure 3.** This graph plots the current–voltage characteristics of the structure shown in figure 2. The chosen value of  $I_c$  merely affects the position of the step in the current–voltage relation.

By solving equations (5) and (6) one obtains the current–voltage characteristic shown in figure 3. The cross-over from the high-sub-gap-conductance region (a) to region (b) occurs when the voltage difference  $\mu_1 - \mu$  exceeds  $|\Delta|$ . The vertical drop (c) occurs when the current  $I$  exceeds  $I_c$ , at which point the value of  $|\Delta|$  given by equation (6) undergoes a first-order transition to zero. Finally, in region (d), the system is normal and exhibits the same above-gap conductance as region (b). To obtain the quasi-self-consistent results of figure 3,  $\Delta_0$ ,  $I_c$ ,  $Z$  and  $k_F$  were imposed quantities. For all energies between  $\mu_1$  and  $\mu$ ,  $R_0$  and  $R_a$  were calculated and  $I$  computed from equation (5). Finally,  $|\Delta|$  was obtained from (6) and the procedure iterated to convergence.

The vertical region (c) of figure 3 corresponds to a region of infinite, negative differential conductance and we now ask whether or not this arises within an exact solution for a finite sample.

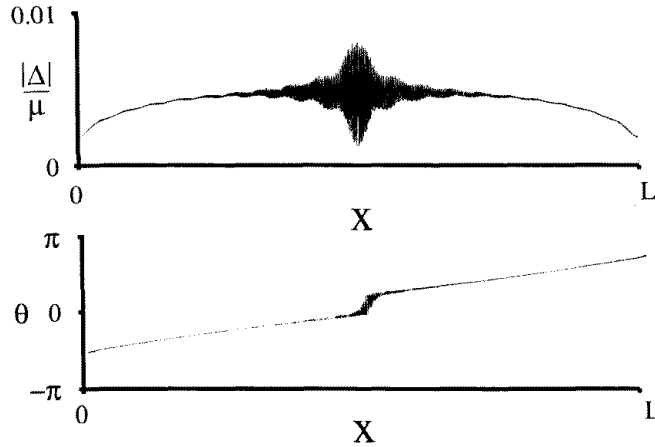


**Figure 4.** The magnitude (top) and the phase (bottom) of  $\Delta(x)$  for an N–S–N structure with two applied voltages  $\mu_1 - \mu_2 = 0$  (thick solid line) and  $\mu_1 - \mu_2 = 0.005\mu$  (thin dashed line).

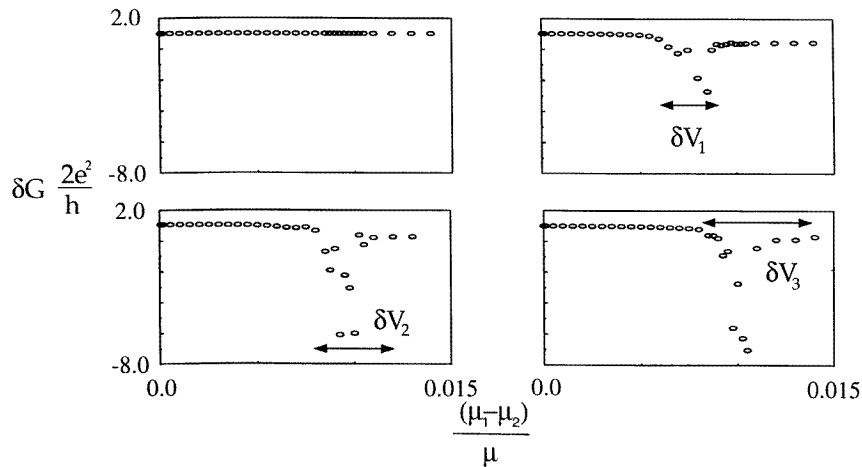
To this end, consider the structure of figure 1 which consists of a scattering region of length  $L = 1500/k_\mu$ , where  $k_\mu = \sqrt{2m\mu}/\hbar$ . When  $Z = 0$  (i.e., no normal scattering potential) we have calculated the self-consistent values of the order parameter, for various applied voltages. Figure 4 shows the profile of  $|\Delta(x)|$  (top) and the order parameter phase  $\theta(x)$  (bottom) for  $\mu_1 - \mu_2 = 0$  (thick solid line) and  $\mu_1 - \mu_2 = 0.005\mu$  (thin dashed line). For finite voltages (thin dashed line) a phase gradient arises naturally from a self-consistent

calculation. As shown in figure 4 the computed phase gradient is almost a constant, even though the order parameter and supercurrent are suppressed near the interfaces. This is consistent with charge conservation, because a finite quasi-particle current penetrates a distance of the order of the superconducting coherence length  $\xi$  into the superconductor.

Figure 5 shows the corresponding results when a normal scattering potential is placed at the centre of the superconductor with  $Z = 1.1$ . The impurity introduces Friedel-like oscillations in the magnitude of the superconducting order parameter [15, 16].



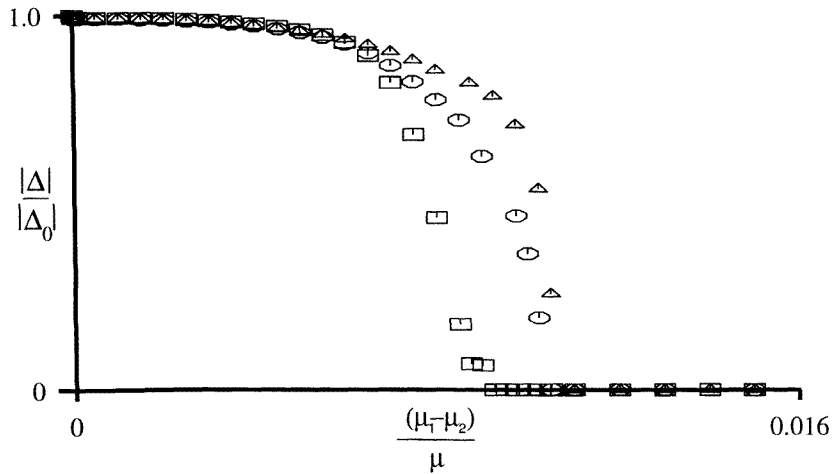
**Figure 5.** The magnitude (top) and the phase (bottom) of  $\Delta(x)$  for an N-S-I-S-N structure for an applied voltage of  $\mu_1 - \mu_2 = 0.005\mu$ ,  $Z = 1.1$ .



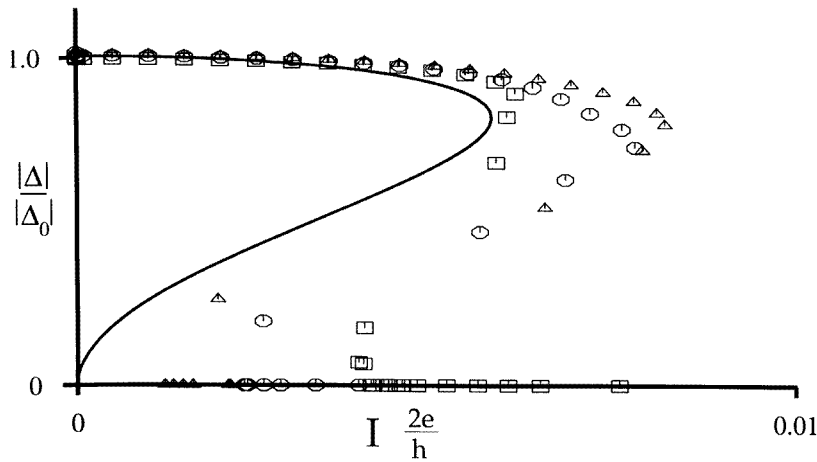
**Figure 6.** Four graphs depicting the differential conductance versus the applied voltage for four different values of  $Z$ :  $Z = 0$  (top left);  $Z = 1.1$  (top right);  $Z = 1.8$  (bottom left);  $Z = 2.6$  (bottom right).

Figure 6 shows the self-consistent differential conductance as a function of the applied voltage for four different values of  $Z$ . For  $Z > 0$  there is a dramatic drop in  $\delta G$  at a voltage

which, as shown in figure 7, corresponds to the critical current of the superconductor and hence to a dramatic fall in the order parameter.



**Figure 7.** A graph depicting the change in  $|\Delta|$  versus the applied voltage for three different values of  $Z$ :  $Z = 1.1$  (squares);  $Z = 1.8$  (circles);  $Z = 2.6$  (triangles).  $|\Delta|$  is defined to be the average value of  $|\Delta(x)|$  over the whole scattering region.



**Figure 8.** A graph depicting the change in  $|\Delta|$  versus the current for three different values of  $Z$ :  $Z = 1.1$  (squares);  $Z = 1.8$  (circles);  $Z = 2.6$  (triangles). The solid line is the G-L function for the order parameter as a function of the supercurrent, given by equation (5).

For completeness, we also show, in figure 8, a plot of the self-consistent value of  $|\Delta|$  versus the self-consistently determined current. The solid line is a plot of the Ginzburg-Landau result (equation (6)). Since the latter is an expression for the supercurrent only, it vanishes when  $|\Delta| = 0$ . In contrast the numerical results yield the total current, which remains finite, even in the limit  $|\Delta| = 0$ .

In contrast with the quasi-self-consistent, infinite negative differential conductance shown in figure 3, the self-consistent calculations of figure 6 show that the conductance of a superconducting dot remains finite. This is a consequence of the smearing of a first-order transition to the normal state, due to the finite size of the dot. Nevertheless the negative conductance has a magnitude which exceeds the quantum of conductance  $2e^2/h$ , despite the fact that the external leads possess only a single scattering channel. This effect arises only for intermediate values of  $Z$ . For  $Z = 0$  the effect vanishes, because for an N–S–N metallic structure with  $\Delta_0/\mu \ll 1$ , the normal state conductance is almost identical to the conductance in the superconducting state. For large  $Z$  (or large  $L/\xi$ )  $I_c$  would be greater than the critical current of the Josephson weak link formed by the delta-function barrier, hence no stationary self-consistent solution can be found.

Although the analysis presented in this paper is restricted to one dimension, we believe that the above effect will carry over to two- or three-dimensional structures with a planar barrier at  $90^\circ$  to the direction of current flow, provided that oscillations on the scale of the Fermi wavelength are ignored. (Such oscillations are neglected by quasi-classical descriptions of N–S interfaces.) In this case the scattering states are of the form

$$\begin{pmatrix} u_n^i(x) \\ v_n^i(x) \end{pmatrix} \chi_i(y, z)$$

where  $i$  sums over all open channels. In the presence of  $M$  such open channels (at  $E = 0$ ), ignoring oscillations on the scale of  $k_F^{-1}$  yields for the superconducting order parameter

$$\Delta(x) = (1/M) \sum_{i=1}^M \Delta_i(x)$$

with

$$\Delta_i(x) = V(x) \sum_{\substack{n>0 \\ \sigma}} (v_n^i(x) u_n^{i*}(x)) \left( \frac{1}{2} - \langle \langle \gamma_{ni\sigma}^\dagger \gamma_{ni\sigma} \rangle \rangle \right). \quad (7)$$

Since the sum over  $n$  is restricted to energies close to  $E = 0$ ,  $\Delta_i(x)$  is almost channel independent and the self-consistent value of  $\Delta(x)$  is almost identical to the one-dimensional result. As a consequence, although the rapid oscillations present in figure 5 will not be present in higher dimensions, we expect that the slower (Tomasch) oscillations will survive and the differential conductance, shown in figure 6, will scale with the number of open channels.

This work is supported by the EPSRC, ISI Foundation and the EC HCM programme. I would also like to thank F Sols, J Sánchez Cañazares, M Leadbeater and R Raimondi for useful discussions.

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