Transport in normal-superconductor-normal structures
with local conservation of current

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Abstract

We study the transport properties of a NSN structure with an insulating barrier at each NS interface. Coherent quasiparticle scattering is assumed and self-consistency is implemented exactly to guarantee local charge conservation. The presence of a finite condensate flow has a greater influence on the transport properties than either the gap depression near the interfaces or the coherent nature of scattering. We find that a nonzero phase gradient causes a shift towards lower voltages of the first peak in the differential conductance and a global enhancement of current. At low currents, we obtain gap profiles near the interfaces that are consistent with the criteria for boundary conditions employed in macroscopic descriptions. The existence of coherent multiple scattering gives rise to a rich structure of resonances that is smoothed out for long superconductors.

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I. INTRODUCTION

Motivated by the recent development of mesoscopic superconductivity, the study of transport in normal-superconductor structures has been the object of renewed attention. Microscopic studies are conventionally performed within the framework of the Bogoliubov-de Gennes (BdG) equations:

\[
\begin{bmatrix}
H_0 & \Delta \\
\Delta^* & -H_0^*
\end{bmatrix}
\begin{bmatrix}
 u_n \\
v_n
\end{bmatrix} = \varepsilon_n
\begin{bmatrix}
 u_n \\
v_n
\end{bmatrix},
\]

where \([u_n, v_n]\) and \(\varepsilon_n\) are the wave function and energy of quasiparticle \(n\). \(H_0\) is the one-electron Hamiltonian referred to the Fermi energy and \(\Delta\) is the pair potential. The BdG equations are based on a mean field Hamiltonian which does not commute with the particle number operator. It has been noted that current conservation is only guaranteed if the BdG equations are solved within a self-consistent scheme, i.e., one in which the gap function \(\Delta(r)\) is required to satisfy the condition

\[
\Delta = g \sum_n u_n v_n^* (1 - 2f_n),
\]

\(g\) being the electron-phonon coupling constant and \(f_n\) the occupation probability.

The requirement of current conservation can be satisfied only if the condensate carries a finite amount of current and for this a nonzero phase gradient is needed: \(\nabla \varphi \neq 0\), with \(\Delta \equiv |\Delta| e^{i\varphi}\). At distances from the scattering region much bigger than the coherence length, the superfluid velocity \(v_s \equiv \hbar \nabla \varphi / 2m\) and the gap amplitude acquire uniform values. Based on this result, a model was developed in Ref. to compute the current-voltage characteristics for several normal-superconductor structures with the simplifying assumptions of asymptotic self-consistency (current is globally conserved) and incoherent multiple scattering (if more than one interface is present). A rich transport behavior was unveiled of which the most salient features are a shift towards lower voltages of the first peak in the differential conductance and an enhancement of current at not very low voltages caused by the greater availability of current carrying scattering channels. Different voltage regimes
appear in the presence of a finite condensate flow, since this creates a distortion in the quasiparticle dispersion relation within the superconductor which makes the various quasiparticle channels open at different voltages. A regime was found in which quasiparticles enter and leave the superconductor only through Andreev transmission and in which current is thus insensitive to the presence of impurities within the superconductor. It was also shown that a state of anisotropic gapless superconductivity can develop for high enough voltages if the temperature is low. Effects due to a finite superfluid velocity are important when the supercurrent is comparable to the bulk critical current. This may occur already at voltages of order $\Delta_0/e$ if the interfaces are transmissive and the superconductor is at most as wide as the semi-infinite normal leads, i.e., if there is no geometrical current dilution in the superconductor. The self-consistent gap near a NS interface with zero current was already studied by McMillan and, more recently, by Bruder in the context of anisotropic superconductivity.

The purpose of this paper is to go beyond the approximations introduced in the model of Ref. and study the nonlinear transport of a NSN structure within a picture in which quasiparticles undergo multiple coherent scattering and current is locally conserved (self-consistency is implemented exactly). In particular, we wish to know which of the transport properties found in Ref. survive in a more accurate description. Like in previous scattering studies of transport through NS structures, we assume that an insulating barrier may exist at the interface contributing $H\delta(x)$ to the one-electron potential $H_0$. The dimensionless parameter $Z \equiv mH/\hbar^2k_F$ is a measure of the barrier scattering strength, since the one-electron reflection probability is $Z^2/(1 + Z^2)$. We are interested in NSN structures which contain two insulating barriers -one at each interface- of strengths $Z_1$ and $Z_2$. By performing a systematic study of the dependence of transport properties on the values of $Z_1$ and $Z_2$, as well as on the length of the superconductor, we extend the work of Martin and Lambert where a similar set of assumptions was employed.

In an asymmetric NSN structure, the distribution of the potential drop between the two
interfaces has to be determined self-consistently, like in the asymptotic model of Ref. 8. Here we determine in addition the exact profile of the pair potential $\Delta(x)$. Consistently with previous work, 8 we find that the position of the first peak in the differential conductance (FPDC) is shifted to lower voltages, because of the existence of a nonzero phase gradient. This effect is more important than the local depression of $\Delta(x)$ or the coherent nature of quasiparticle scattering. Due to the coherent multiple scattering, a structure of resonances develops which gives rise to an oscillatory behavior of $dI/dV$ as a function of voltage and length (see Figs. 4 and 5). The results obtained from the model of incoherent scattering and asymptotic self-consistency are recovered qualitatively for structures where the superconductor is much longer than its coherence length.

II. THE MODEL

We wish to solve the BdG equations (1) self-consistently within the context of a onedimensional model. The resulting gap (2) will in general be space dependent. At a given energy, a scattering problem has to be solved which is defined by Eq. (1) with $H_0$ describing a NSN structure with insulating barriers at the interfaces. Quasiparticle scattering states are labeled by the incoming channel $\alpha$. Thus, index $\alpha$ indicates the lead (left or right) and the type (electron or hole) of the initial quasiparticle state. We can exploit the fact that only wave vectors in a small interval around $\pm k_F$ are important, and linearize the one-electron Hamiltonian around the two Fermi points. In momentum representation,

$$\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}(\pm k_F + \kappa)^2 \simeq E_F \pm \frac{\hbar^2 k_F \kappa}{m} = -E_F \pm \frac{\hbar^2 k_F}{m} \kappa.$$  \hspace{1cm} (3)

Therefore, instead of $H_0 = (\hbar^2/2m)(-d^2/dx^2) - E_F$, we can write

$$H_0 \simeq \pm i \frac{\hbar^2 k_F}{m} \frac{d}{dx} - 2E_F,$$  \hspace{1cm} (4)

in the vicinity of $\mp k_F$. For the numerical resolution, the BdG equations are discretized within the superconductor $S$, so that only a finite set of positions $x_i = iL/N$ (with $i = 0, 1, ..., N$)
are considered, with a uniform spacing $\delta = L/N$. Within the interval $[x_i - \delta/2, x_i + \delta/2]$ the solution of Eq. (1) can be written as a sum of quasiparticle plane waves, $\sum_\beta t_{i\alpha}^\beta e^{ik_i^\beta x}[u_i^\beta, v_i^\beta]$ which are solutions for the “uniform” gap $\Delta(x_i)$. This is a safe procedure if $\delta$ is chosen much smaller than the superconducting coherence length $\xi_0 = \hbar v_F/\pi \Delta_0$, which is the typical length scale for gap variations. At each point and energy, there are four possible quasiparticle states labeled by $\beta$. The components at $i + 1$ are obtained in terms of the components at $i$ through a $4 \times 4$ transfer matrix that is determined by wave function matching at $x = (x_i + x_{i+1})/2$. When a linearization scheme is adopted, the $\pm k_F$ branches do not couple within the superconductor (only Andreev reflection or normal transmission can occur) and the transfer matrix at each point is box-diagonalized into two $2 \times 2$ matrices. Right at the interfaces ($x = 0$ and $x = L$) normal reflection and thus branch mixing occurs, and in those points the transfer matrix is also determined by standard matching techniques. The global transfer matrix is obtained by compounding the individual transfer matrices.

Once the scattering quasiparticles have been calculated, the gap is determined from Eq. (2). Due to normal reflection at the interfaces, a quasiparticle $n$ has in general components from both $\pm k_F$ branches. This gives rise to irrelevant oscillations in $\Delta(x)$ on the scale of the Fermi wavelength, which we smooth out by introducing only intra-branch interference terms in the gap equation (2). Once self-consistency has been achieved, the resulting description does conserve charge and the electric current must be uniform.

Self-consistency is implemented as follows. The input parameter is the difference in chemical potentials between the quasiparticles coming from the left and the right normal leads. The desired output is the resulting current. The pair potential profile $\Delta(x)$ and the chemical potential at the superconductor $\mu_S$ are treated on the same footing, as parameters that are progressively adjusted to achieve convergence. In the first scattering calculation, some guess values for the $\Delta(x)$ profile and $\mu_S$ are introduced. From the global transfer matrix we obtain the quasiparticle scattering states, and from them the current in the normal leads. For the following iteration, the gap at each point is obtained from Eq. (2)
and the superconductor chemical potential is adjusted to make the currents in both leads equal. Self-consistency is achieved when $\Delta(x)$ and $\mu_S$ converge and the current in the two leads is the same within tolerable errors.

The main simplifications that we have introduced are: (i) Use of a one-dimensional model, which we expect to yield qualitatively correct physics in structures with planar interfaces where mode mixing is not important. (ii) The voltage drop takes place entirely at the interfaces and the chemical potential within the superconductor is uniform. (iii) There is no proximity effect ($g(x) = 0$ in the normal metal). A similar set of approximations were employed in Ref. with the difference that no linearization procedure was implemented there. Relaxation of (ii) and (iii) may yield interesting physics, but here we want to focus on the effect of a nonuniform, complex $\Delta(x)$.

III. RESULTS

There are two main ways in which local current conservation can affect the transport properties of a NSN structure. One is the induction of a nonzero phase gradient, which has already been mentioned. The second effect has to do with the local depression of the gap near the interface, which is a direct consequence of self-consistency that already occurs at $v_s = 0$. From the work of Refs. we have some understanding of the effect of flow and now we wish the explore the effect of gap depression at the interface. In Fig. 1 we plot for comparison the Andreev reflection probability as a function of the quasiparticle energy for gap profiles with a step-like structure (solid lines) and with a local, smooth depression shown in the inset (dotted lines). The profiles have been obtained by truncating (and matching with a uniform gap) the self-consistent gap of a NSN structure with zero current. Thus, there is no flow effect in any of the two cases. A similar study has been performed by van Son et al. introducing phenomenological gap profiles with a proximity effect. The influence on scattering of the local gap reduction is small in the cases of low and high $Z$, but it is appreciable for intermediate $Z$. At energies $E \lesssim \Delta_0$, Andreev reflection (AR) is
enhanced for $Z = 0.5$ because it takes place in three distinct (albeit coherent) steps: the electron is first normally transmitted, then it is Andreev reflected as it finds a higher gap, and finally the emerging hole is normally transmitted. AR at the smooth gap increase takes place with probability very close to unity. On the other hand, the two normal transmission (NT) processes are more probable than direct AR (since this requires the simultaneous transmission of two particles), which is the only possibility when $E < \Delta(x = 0)$. Thus, by being decomposed into three processes of higher probability, AR takes place more easily. The effect of gap depression is very small at $Z = 0.1$ because direct AR already has a high probability. For high $Z$, the gap depression is small and thus it cannot have important consequences.

In Figs. 2 and 3, we plot the gap amplitude $|\Delta|$ as a function of position and voltage for two asymmetric NSN structures: $(Z_1, Z_2) = (0.1, 0.5)$ (Fig. 2) and $(2, 0.5)$ (Fig. 3). Here, $Z_1$ and $Z_2$ are the barrier parameters at $x = 0$ and $x = L$, respectively. In both cases, $L = 8\xi_0$. At low voltages, $|\Delta|$ is strengthened if the barrier is thick, while it is more strongly depressed near a transmissive interface. This is in qualitative agreement with the Ginzburg-Landau result for the boundary conditions describing the interface between a superconductor and an insulator or a normal metal. At a transmissive NS interface, the order parameter must be zero, while at the interface with an insulator (here represented by a high $Z$ interface), it is the derivative of the order parameter what must vanish. We see again that the physics obtained from a self-consistent description at zero temperature is qualitatively similar to that which is derived from the Ginzburg-Landau approximation near the critical temperature. As the voltage increases, it drops mostly at the more reflecting interface, where a greater gap reduction takes place because of the stronger presence of quasiparticles. In fact, Fig. 2 shows the rather counterintuitive feature that $|\Delta|$ can even become smaller at the more reflecting interface, in marked contrast with the zero voltage behavior.

Upper Fig. 4 shows the differential conductance $dI/dV$ as a function of voltage for several structures as obtained from different types of calculations. Thick and solid lines
have been obtained with exact and asymptotic (see Ref. 8) self-consistency, respectively. The
other three lines have been obtained from uniform phase calculations, in the spirit of Ref. 13:
The dotted (dashed) line corresponds to incoherent (coherent) scattering, while the long-
dashed line results from a coherent scattering calculation performed with the self-consistent
gap profile of the zero current case: \( \Delta(x, V = 0) \). In all cases, \( Z_2 = 0.5, L = 8\xi_0 \), and
\( T = 2 \) K have been taken, with superconductor material parameters corresponding to those
of Pb (\( T_c = 7.2 \) K). The lower part of Fig. 4 shows the relevant energies of the problem at
the midpoint \( x = L/2 = 4\xi_0 \) corresponding to the exactly self-consistent calculation:
\(|\Delta|\) (dotted), \( \Delta^+ = |\Delta| \pm \hbar q v_F \) (dashed), and the voltage difference at each interface (solid).

The first peak in the differential conductance (FPDC) occurs when \( eV \) reaches \( \Delta^- \),
and its position is very sensitive to the existence of finite superconducting flow. This is
particularly clear in the case of the symmetric (\( Z_1 = 0.5 \)) NSN structure. The lowering
of the FPDC is less marked in the \( Z_1 = 0.1 \) case because the asymmetric voltage drop
tends to mask the effect. Finally, for \( Z_1 = 2 \), the FPDC is barely shifted, because of a
global reduction of current caused by poor transmittivity. As compared with calculations
based on asymptotic self-consistency, implementation of local self-consistency and coherent
quasiparticle scattering displaces the FPDC position only slightly, and tends to increase the
current.

The existence of coherent multiple reflection at the interfaces gives rise to a structure
of resonances that is clearly appreciated in the plot of \( dI/dV \) vs. voltage. The oscillatory
behavior of the differential conductance predicted by coherent scattering calculations
contrast with the less structured curves obtained from the assumption of incoherent scat-
tering. These resonances are very efficient at carrying current because they are made of
quasi-bound states in which the quasiparticles are mostly Andreev reflected at the inter-
faces. Thus, for instance, a right-moving electron is Andreev reflected as a left-moving hole,
which in turn is reflected as a right-moving electron, and repetition of the process results in
a strong net electron current to the right. These oscillations are very similar in nature to
the Tomasch oscillations occurring in tunnel junctions and also occur in other transport contexts involving coherent Andreev reflection.

The period of the oscillations in $dI/dV$ is strongly sensitive to the total superconductor length $L$. Actually, for a superconductor with constant $\Delta = \Delta_0$, one would expect to have resonances at energies

$$E_n = \Delta_0 \left[ 1 + \frac{(n - 1/2)^2 \pi^2 \xi_0^2}{L^2} \right]^{1/2},$$

which is obtained from requiring $k_+ - k_- = (2n - 1)\pi/L$ ($k_{\pm}$ are the two possible solutions to $\varepsilon(k) = E$ in the $+k_F$ branch, $\varepsilon(k)$ being the quasiparticle dispersion relation). In our case, Eq. (5) is not exactly fulfilled because of the effect of $v_s \neq 0$ on the pair potential. Nevertheless, Fig. 5 shows that the separation between peaks decreases with increasing $L$, with a first peak that is not very sensitive to the length (see inset). The spacing between peaks depends also on the values of $Z$ (not shown) because of the effect that these have on the effective gap amplitude.

IV. CONCLUSIONS

We have performed a self-consistent scattering calculation of nonlinear transport through asymmetric NSN structures. By introducing local current conservation and coherent scattering of quasiparticles, we have gone beyond the model employed in Refs. 7, 8, where incoherent multiple scattering and global current conservation was assumed. Comparison of the results obtained from the two different models allows us to identify the most robust physical features which are likely to survive in realistic scenarios. In both models we have obtained a lowering of the voltage threshold for quasiparticle transmission (as signaled by the first peak in the differential conductance) and a global enhancement of current caused by the increased availability of charge-transmitting scattering channels. Both effects are directly related to the presence of a nonzero superfluid velocity in the condensate.

In general, the self-consistent gap does not have a uniform amplitude. Linearization of the BdG equations around the two Fermi wave vectors automatically washes out any spurious
spatial dependence on the scale of the Fermi wavelength, and only the relevant physics occurring at the scale of the coherence length is preserved. The gap amplitude $|\Delta(x)|$ tends to decrease with increasing voltage and is locally depressed in the vicinity of the interface with the normal lead. In the presence of a strongly reflecting insulating barrier the depression is weak and $|\Delta|$ drops abruptly to zero at the interface (no proximity effect is assumed). By contrast, if the interface is transmissive, the gap amplitude drops smoothly from its bulk value to a very small value right at the interface. This result is consistent with the criterion for boundary conditions employed in macroscopic, Ginzburg-Landau descriptions. However, we have found that the presence of a nonequilibrium population of quasiparticles may alter this picture qualitatively.

Quasiparticle multiple scattering is responsible for the existence of resonances within the superconductor. These quasibound states are very efficient current carriers, since they consist mostly of electrons that are Andreev reflected at the interfaces, or vice versa. Whenever the voltage reaches a threshold level that permits transmission through a new resonance, there is a quick rise in the current, hence the nonmonotonous dependence of the differential conductance on the applied voltage (see Figs. 4 and 5). We have found that agreement with incoherent scattering calculations tends to improve as the superconductor length becomes large compared with the coherence length, because in that case the structure of resonances is smoothed out.

We end this article by pointing out some remaining challenges that should be addressed in future scattering studies of current conserving transport. Self-consistency should be extended to include the Coulomb interaction term, since voltage variations due to charge pileup at the barriers may be comparable to the gap if the interface is appreciably reflecting. Most important, it would be desirable to understand how the transport properties discussed here and in previous references are affected by the presence of many modes which can mix at the interface and by collisions with impurities in the superconductor. Finally, it will be of interest to understand how transport is modified by the existence of a proximity effect in
the normal lead.

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REFERENCES

1 For an updated overview, see Mesoscopic Superconductivity, Proc. of the NATO-ARW, F.W.J Hekking, G. Schön, D.V. Averin, eds. (North-Holland, Amsterdam, 1995).

2 P.G. de Gennes, Superconductivity of Metals and Alloys (Benjamin, New York, 1966).

3 A. Furusaki and M. Tsukada, Solid State Commun. 78, 299 (1991).

4 P.F. Bagwell, Phys. Rev. B49, 6841 (1994).

5 F. Sols and J. Ferrer, Phys. Rev. B49, 15913 (1994).

6 J. Ferrer, Ph.D. Thesis, Universidad Autónoma de Madrid (1990), unpublished.

7 J. Sánchez-Cañizares and F. Sols, J. Phys.: Condens. Matter 7, L317 (1995).

8 J. Sánchez-Cañizares and F. Sols, Phys. Rev. B 55, 531 (1997).

9 J. Sánchez-Cañizares and F. Sols, J. Phys.: Condens. Matter 8, L207 (1996).

10 R.A. Riedel, L-F. Chang, and P.F. Bagwell, Phys. Rev. B54, 1 (1996).

11 W.L. McMillan, Phys. Rev. 175, 559 (1968).

12 C. Bruder, Phys. Rev. B41, 4017 (1990).

13 G.E. Blonder, M. Tinkham, T.M. Klapwijk, Phys. Rev. B25, 4515 (1982).

14 A. Martin and C.J. Lambert, Phys. Rev. B51, 17999 (1995).

15 P.C. van Son, H. van Kempen, and P. Wyder, Phys. Rev. B37, 5015 (1987).

16 I. Zapata and F. Sols, Phys. Rev. B53, 6693 (1996).

17 W.J. Tomasch, Phys. Rev. Lett., 15, 672 (1965).

18 N.K. Allsopp and C.J. Lambert, Phys. Rev. B50, 3972 (1994).
FIG. 1. Andreev reflection at a NS interface with different insulating barriers for a stepwise (solid line) and self-consistent (dotted line) pair potential. Insets show the self-consistent pair potentials employed in the calculations.
FIG. 2. Amplitude of the self-consistent pair potential for a NSN structure with $Z_1 = 0.1$ (at $x = 0$) and $Z_2 = 0.5$ (at $x = 8\xi_0$) as a function of position and applied voltage. A temperature of $T = 2$ K (for $T_c = 7.2$ K) has been taken.
FIG. 3. Same as Fig. 2 for $Z_1 = 2$ and $Z_2 = 0.5$. 
FIG. 4. NSN structure. $Z_2 = 0.5$ and data of Pb for S have been taken in all cases. Temperature is $T = 2$ K while $T_c = 7.2$ K. The upper curves show the differential conductance calculated with exact (thick solid line) and asymptotic self-consistency (thin solid). The other three lines result from calculations with a zero phase gradient: Dotted (short-dashed) line corresponds to incoherent (coherent) scattering with a stepwise pair potential, while the long-dashed line corresponds to a coherent scattering calculation performed with a zero-current gap. The lower curves show the relevant energies (in units of $\Delta_0$) of the problem in the exact calculation: Voltage drops at each interface (solid), magnitude of the order parameter $|\Delta|$ (dotted), and of the $\Delta_+$ and $\Delta_-$ thresholds (dashed) evaluated at $x = L/2 = 4\xi_0$. 
FIG. 5. $dI/dV$ vs. $V$ for the $Z_1 = 0.5$ case of Fig. 4 for different superconductor lengths: $L = 8\xi_0$ (solid), $L = 12\xi_0$ (long-dashed), $L = 16\xi_0$ (short-dashed), and $L = 24\xi_0$ (dotted). Inset: Positions of the various resonance peaks as a function of the superconductor length.