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LETTER TO THE EDITOR

Self-consistent current–voltage characteristics of normal–superconductor interfaces

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Abstract. We study the nonlinear transport properties of NS (normal–superconductor) and NSN structures by means of a self-consistent microscopic description. A nonzero superfluid velocity causes the various quasiparticle channels within the S to open at different voltages. The gap reduction is very sensitive to the details of quasiparticle scattering. At low temperatures, superconductivity, sometimes in a peculiar gapless form, may survive up to voltages much higher than $k_B T_c/e$. The minimum voltage for quasiparticle transmission is shown to decrease strongly with temperature and with the transmittivity of the barrier.

During the last few years, there has been a renewed interest in the transport properties of structures that involve both normal and superconducting elements. This research has been largely motivated by the study of mesoscopic superconductivity, whose characteristic feature is the phase coherent propagation of quasiparticles. Due to its fundamental character, the normal–superconductor (NS) interface has been the object of especial attention, and a number of transport anomalies have been associated to the existence of phase coherent Andreev reflection [1]. These investigations have been accompanied by a revived interest in related questions such as the role of self-consistency in microscopic descriptions based on the resolution of the Bogoliubov–de Gennes equations [2]

$$\begin{bmatrix} H_0 & \Delta \\ \Delta^* & -H_0^* \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix} = \epsilon_n \begin{bmatrix} u_n \\ v_n \end{bmatrix}. \quad (1)$$

Here, H_0 is the one-electron Hamiltonian, Δ is the gap function, and (u_n, v_n) and ϵ_n are, respectively, the normalized wave function components and the energy of the quasiparticle n . Self-consistency requires

$$\Delta = g \sum_n u_n v_n^* (1 - 2f_n) \quad (2)$$

where g is the coupling constant and $\{f_n\}$ are the occupation probabilities. The implementation of self-consistency is especially important in transport studies, since it guarantees the conservation of electric current [3, 4, 5]. In a perfect one-dimensional superconductor, uniform current carrying solutions are of the form [2]

$$\Delta(x) = |\Delta| e^{i2qx}. \quad (3)$$

In equilibrium, $|\Delta|$ is a decreasing function of q , with a critical current above which $|\Delta| = 0$ [2, 4, 6]. Self-consistency is also essential to the understanding of the crossover from the Josephson effect to bulk superconducting flow [5]. A smooth crossover is possible thanks

to the existence of uniform and solitonic (with a local gap depression) configurations [5, 7]. For scattering structures, the use of scattering quasiparticle channels compatible with (3) is sufficient to guarantee asymptotic self-consistency [8, 9].

The studies mentioned above either neglect self-consistency or assume equilibrium of quasiparticles. These may be reasonable assumptions in specific contexts, namely, at low voltages (assumption of equilibrium) or for currents much smaller than the critical current of the perfect superconductor (neglect of self-consistency). However, a theoretical description that includes both self-consistency and nonequilibrium effects is mandatory in transport problems involving high applied voltages and large superconducting current densities. In this letter, we make a first step in this direction. First, we generalize the classic scattering study by Blonder and coworkers [10] on the NS interface by including the effect of self-consistency. We will see that this inclusion introduces major changes in the I - V characteristics, but we will also argue that the most spectacular of them are not observable in practice because of the ultimate presence of a second normal lead in any real experiment [11]. For this reason, we extend our analysis of the NS interface to the study of an NSN structure. We compound the two interfaces by assuming incoherent multiple scattering by the two barriers. This simplification has the advantage that it permits us to focus on the properties arising specifically from the combination of self-consistency and the superposition of two interfaces. In this sense, we expect our predictions to be even more robust than those we would have inferred from coherent scattering descriptions, since these might be dependent on fine, not easily reproducible details of the scattering process. Therefore, the realization of the physics discussed in this paper does not require extremely small structures or very low temperatures. The only essential requirement is that, due to the application of high voltages, and in the absence of dilution effects, the superconductor is forced to carry large currents. The possible role of impurities will be analysed in a future paper [9].

Instead of using a locally self-consistent description, we have assumed that the gap is of the form (3) everywhere in the superconductor and zero in the normal lead. This assumption simplifies the numerics considerably and underlines *the main effect of self-consistency*, which is *the introduction of a nonzero superfluid velocity* $v_s \equiv \hbar q/m$ *in the current carrying configurations*. In our scattering approach, we assume that quasiparticles are sent through the incoming channels of the semi-infinite leads with chemical potentials that differ by eV . Then, we look for self-consistent values of $|\Delta|$ and q satisfying equations (1)–(3) and asymptotic current conservation. We wish to emphasize that *the occupations* $\{f_n\}$ *are those of a nonequilibrium population*. The existence of a nonzero v_s has the major implication that the energy thresholds for propagation across the superconductor are modified, as shown in the insets of figure 1(b). The minimum energy to excite a quasiparticle in the positive ($+k_F$) and negative ($-k_F$) branches becomes Δ_+ and Δ_- , respectively, with $\Delta_{\pm} \equiv |\Delta| \pm \hbar v_F q$. $|\Delta|$ can in turn be suppressed by current, in a manner that is very sensitive to the details of the scattering process.

At zero temperature, electrons with energy $0 < E < eV$ are injected from the normal side onto the NS interface. At low voltages ($eV < \Delta_-$), normal and Andreev reflection (AR) are the only scattering mechanisms. In a AR process, a hole is reflected on the N side and two electrons are transmitted to the superconductor forming a Cooper pair. Thus, one AR event contributes a charge $2e$ that is transported by the condensate. As the voltage is raised, q increases and, when $eV > \Delta_-$, Andreev transmission (AT) also becomes possible: one electron is transmitted to the superconductor, forming a Cooper pair and creating a quasihole. The amplitude for AT is proportional to r^*t , where $r(t)$ is the one-electron reflection (transmission) coefficient [10]. One AT event contributes a net charge of e to

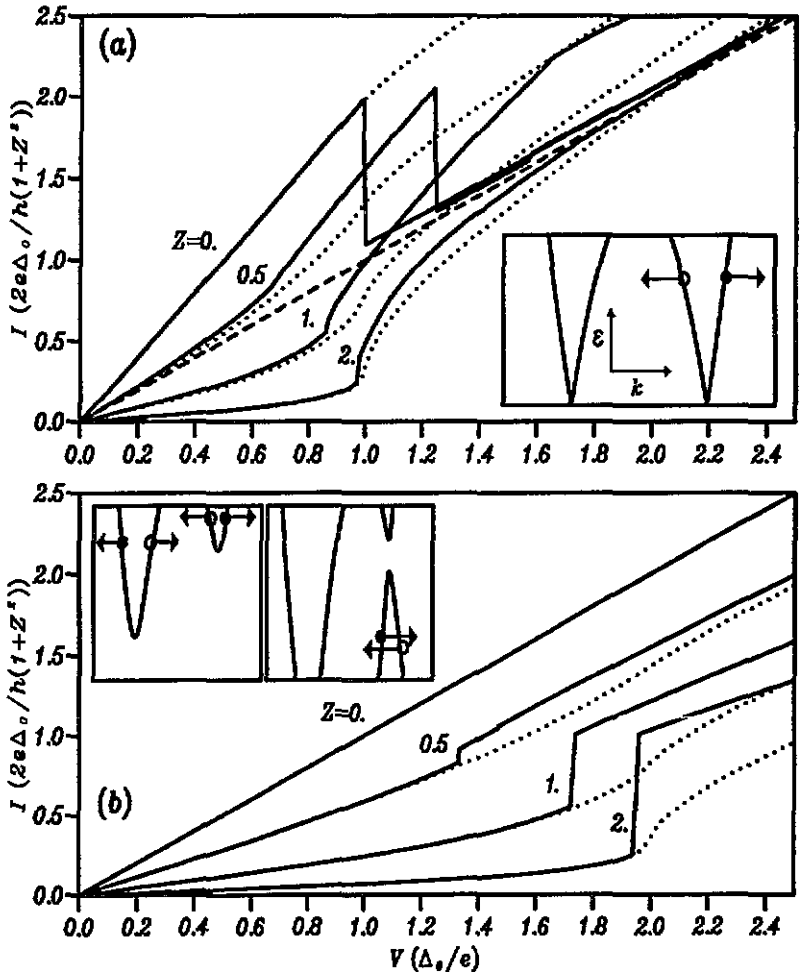


Figure 1. Solid lines show the self-consistent I - V characteristics of an NS (a) and an NSN (b) structure, for four values of Z . Dotted lines show the results from a non-self-consistent calculation [9]. The dashed line in (a) gives the NN result. Insets: schematic quasiparticle dispersion relation, $\epsilon(k)$, in the (a) normal and (b) superconducting leads. The right-hand inset in (b) shows gapless superconductivity. Filled (empty) circles indicate electron- (hole-) like propagation.

the current, $2e$ going to the condensate and $-e$ to the quasiparticle part. Thus, AT is less efficient than AR in that, for the same contribution to the total current, it displaces the condensate twice as much and thus costs more free energy. We remark that there is a range of voltages in which AT is the *only* quasiparticle transmission mechanism. By contrast, in a non-self-consistent description, the AT and normal transmission (NT) channels have the same voltage threshold [10].

As V and q continue to increase, the threshold Δ_- becomes negative. In some cases, and especially at low temperatures, a type of *gapless superconductivity* (GS) with peculiar properties may survive. As shown in the right-hand inset of figure 1(b), the quasiparticles that are hidden below the $\epsilon = 0$ line in the negative branch re-emerge with positive energy in the opposite branch. For each quasiparticle n that satisfies equation (1), there is another

solution n' with energy $\epsilon_{n'} = -\epsilon_n$ and wave components $u_{n'} = -v_n^*$ and $v_{n'} = u_n^*$ [2]. Creating n' , σ is equivalent to destroying n , $-\sigma$ (σ is the spin), and one is free to employ the n or n' description [9]. The conventional choice is that which makes the energy positive, so quasiparticles are rare at low temperatures. Following this convention, a quasiparticle n that acquires negative energy when GS is reached must pass to be described by its n' counterpart. In the GS regime, low-energy electrons coming from the N side can be normally transmitted as quasidelectrons in the lower positive branch. Being of the n' type, this quasiparticle state has some unusual properties. Since $u_n v_n^* = -u_{n'} v_{n'}^*$, it is clear from equation (2) that the presence of n' -type quasiparticles tends to *cancel* the effect of conventional (n -type) quasiparticles. In a standard scenario without GS, the occupation of a quasiparticle state tends to decrease the value of the gap because the factor $(1 - 2f_n)$ changes sign and tends to cancel the contribution from unoccupied states. In the presence of GS, the group of n' -type quasiparticles acts in the opposite way. In front of already existing n -type quasiparticles, these unconventional quasiparticle states *tend to depress the gap if they are empty and contribute to reinforce superconductivity if they are occupied*.

In the spirit of [10], we have modelled the NS interface with a step function gap and a one-electron potential barrier $V_0 \delta(x)$ of effective strength $Z \equiv V_0 / \hbar v_F$. The self-consistent current-voltage characteristics are computed for different values of Z . Except for in a final prediction, we focus on the zero-temperature case. We remark that it has been checked that the self-consistent solutions with $|\Delta| \neq 0$ have *lower free energy* than the trivial solutions with zero q and $|\Delta|$. We have taken a bandwidth of $E_F = 5$ eV, a cut-off energy of $\hbar\omega_D = 0.1$ eV for equation (2), and a zero-temperature, zero-current gap of $\Delta_0 = 1$ meV. This yields a critical temperature of $T_c = 6.6$ K. In figure 1(a), we show the self-consistent I - V characteristics for an NS interface ($e > 0$). Non-self-consistent results [10] are also shown for comparison.

A detailed understanding of the physics behind the I - V curves shown in figure 1(a) would require information on the dependence of $|\Delta|$, v_s , and the quasiparticle current on the applied voltage, which will be presented elsewhere [9]. Here, we only wish to note that, as the voltage increases, the first rise in the current is due to the opening of the AT channel (except in the $Z = 0$ case, where it is forbidden because $r = 0$). The sharp decrease in I for $Z = 0$ and 0.5 is due to the onset of the GS regime, where normal quasiparticle transmission into the unconventional branch begins to dominate, bringing down the value of the conductance from close to two (in units of $2e^2/h$), typical of a transmissive NS interface, to near unity, as corresponds to reflectionless normal transport. This rather spectacular feature is however not likely to be measurable in practice, since it would be destroyed by the presence of a second normal lead. For example, in the transparent case, this second interface must send the value of the low- V differential conductance back to its natural limit of one. On the other hand, nonequilibrium effects that depend essentially on the total depopulation of incoming channels from the S side can hardly be manifest when a second normal lead sends quasiparticles from the opposite side. These considerations motivate our study of the NSN structure, for which we assume identical barriers and incoherent multiple scattering. By symmetry, the potential difference will be $V/2$ at each interface, and the flux of incoming electrons from the left N lead will be mirrored by the flux of incoming holes from the right N lead.

In figure 1(b), we show the resulting $I(V)$ curve for an NSN structure. Non-self-consistent results obtained with analogous scattering assumptions are also shown. Comparison with figure 1(a) does indeed reveal major changes. If $Z = 0$, the presence of a superconducting segment does not affect the conductance, since it adds nothing to perfect transmission. Being as $r = 0$, AT is inhibited. When $v \equiv eV/\Delta_0 = 2$, the system reaches

GS, but, remarkably, $|\Delta|$ can be shown to remain unaffected [9]. This happens because, when the unconventional branch emerges, *its two states are filled with very high probability and thus do not contribute to depress the gap*. This surprising behaviour contrasts markedly with that expected for situations in which quasiparticles are in equilibrium. In such cases, $|\Delta|$ is predicted to decrease very quickly as Δ_- becomes negative [4, 6]. Here, a strong departure from equilibrium gives rise to an effective translational invariance that explains the small sensitivity of $|\Delta|$ to high voltages.

For thicker barriers, we see that, in a non-self-consistent calculation, the jumps in the current are much smoother and occur at higher V . For $Z = 0.5$, the AT channel opens for $v \simeq 1.3$, causing a small decrease in $|\Delta|$ [9], and GS sets in for $v \simeq 1.8$. The onset of GS is almost inconsequential for the gap and total current behaviour, for reasons similar to those of the transparent case. We conclude that, for NSN structures with low Z , the voltage is inefficient in destroying superconductivity, although this may remain quite marginal (in the GS regime, the actual current carried by the condensate is a small fraction of the total current).

For $Z = 1$ and 2, the system bypasses the only-AT regime and jumps directly to GS for $v \simeq 1.7$ and $v \simeq 1.9$, respectively. We attribute this behaviour to the energetic cost of opening two AT channels. The superconductor finds it more favourable to carry charge through the NT channel by going gapless. An important effect is that multiple normal reflection increases the residence time of the injected quasiparticles. At high Z , one can prove by invoking unitarity [9] that all the effective occupations within S tend to $\frac{1}{2}$ (two of the four incident channels are empty), as opposed to the low- Z case (see above) in which conventional (unconventional) channels are occupied with low (high) probability. This effect causes $|\Delta|$ to decrease with increasing Z , in marked contrast with the behaviour found for the NS case [9].

The above discussion shows that, for the values of Z considered, superconductivity can exist at least up to voltages of order $5k_B T_c/e$. Internal thermalization of quasiparticles would tend to destroy this effect. In this sense, we can state that *the survival of superconductivity at high voltages is a nonequilibrium effect*.

We would like to end this discussion with a few comments about the effect of temperature and dimensionality. Provided the superconductor can still be treated as quasi-one-dimensional (width much smaller than coherence and penetration lengths), the effect of many channels is that of requiring higher q to observe similar effects, since high-lying channels have a smaller effective longitudinal Fermi velocity. Also, the presence of many channels effectively breaks the translational invariance we found for very transmissive barriers [9]. As a consequence, the survival of superconductivity at high voltages is considerably weakened, in accordance with the behaviour found in semiclassical nonequilibrium superconductivity [12]. Apart from smoothing the structure of the $I(V)$ curves, the main effect of temperature is that of bringing down the scale of gap energies. With smaller gaps, the condensate needs higher values of q and the result is that *self-consistency effects are even more important. A major consequence is that, as the voltage increases, the thresholds for the novel regimes discussed above are anticipated*. Figure 2 shows that the voltage threshold for the onset of AT, V_{AT} , which determines the first peak in the differential conductance, is a decreasing function of temperature, even when measured in units of the zero-current gap $\Delta_0(T)$. One may also note that V_{AT} increases with Z , due to a global reduction of v_S .

In conclusion, we have performed a self-consistent calculation of the nonlinear transport properties of NS and NSN structures. A major effect of self-consistency is that of forcing the current carrying superconductor to have a nonzero superfluid velocity. This causes the

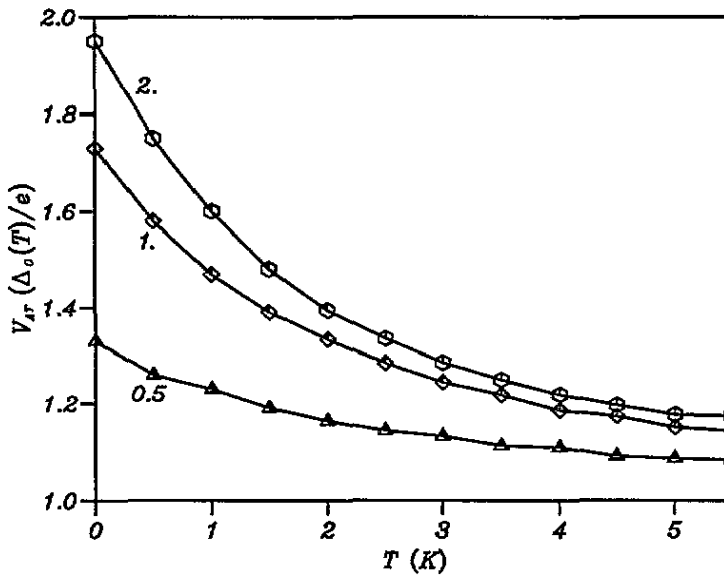


Figure 2. Position of the first peak in the differential conductance (caused by the onset of Andreev transmission), in units of the zero-current gap, plotted as function of temperature for $Z = 0.5, 1,$ and 2 .

various quasiparticle channels to enter into action at different voltages. The study of the NS interface has served to identify the scattering processes separately and has allowed us to understand in detail the properties of the more realistic NSN system. The gap amplitude is depressed by the flow of current in a way that is very sensitive to the details of the scattering problem. An important nonequilibrium effect is that, at low temperatures, a type of gapless superconductivity may survive up to voltages considerably greater than $k_B T_c/e$, although this effect may be weakened in the presence of many channels. The onset of Andreev transmission is signalled by a peak in the differential conductance whose position relative to the zero-current gap has been predicted to decrease with temperature and with the transmittivity of the barrier.

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Note added. After this work had been completed, we learned about the content of [13], where a related NSN model has been studied. In [13], one interface is always transmissive and multiple phase coherent scattering is assumed. In spite of these differences, the model studied by Martin and Lambert [13] displays some common robust features like the splitting of voltage thresholds and the depression of the gap.

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