Subgap resonances and conduction channels in mesoscopic superconducting devices.

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Peaks associated to multiple Andreev reflections have been used to identify the number of conduction channels, and their transmittivity, in mesoscopic superconducting junctions. We analyze the influence of the detailed shape of each channel, and the number of weak links within it, on the final results. Connexions with the statistical interpretation of conductance histograms is also made.

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Many experiments show that the conductance of narrow constrictions between different metals is quantized. The nature of the structures which give rise to this effect is not well known. The forces transmitted through the constriction show discontinuous jumps correlated with the conductance steps, suggesting that abrupt atomic rearrangements give rise to the conductance steps. Direct observations show irregular, and even amorphous structures near the contact.

The simplest explanation of the observed quantization describes the region near the constriction in terms of a fixed number of almost fully open channels. Such a picture is consistent with models in which the constriction is described in terms of nearly free electrons. Related schemes have been used to describe the force oscillations observed experimentally. Statistical averages based on models where the connexion between the channels within the constriction and the electrodes are allowed to vary randomly, support this picture. A model of an n-channel constriction coupled to N-channel electrodes, shows the desired features, when n ≪ N, and the reflection and transmission of electrons from the electrodes are taken to be random matrices.

An alternative picture, based on local properties of the atoms at the constriction has also been put forward. The conductance is defined using localized wavefunctions at the atoms within the constraint. When the constriction narrows to a single atom at some point, conductances near a single quantum are obtained. The bands of metals such as Pb or Al arise, basically, from the hybridization of s and p atomic orbitals, while those of Na or Au are mainly derived from s orbitals. Hence, the number of channels through a one atom constriction in a nearest neighbor tight binding scheme is at least three for Pb or Al, while it is one for Au.

These two pictures can be adapted to give similar results for the total conductance of the constriction, at least when a single quantum is observed. The properties of superconducting constrictions, however, are expected to differ. The I-V characteristics of a superconducting constriction described by a single channel with one barrier are significantly different from those of three or more channels, even if the total conductance in the normal state is the same. The Andreev spectrum below the superconducting gap has a much richer structure in the second case. Experimental results show, very conclusively, that the Andreev spectrum in Al and Pb is better fitted by a model of three or more superconducting channels in parallel, with a suitably adjusted transmission coefficient. Current investigations try to elucidate if a similar distinction can be made in other quantities which do not depend linearly on the total conductance, such as the critical current or the noise spectrum.

We will now focus on the difference between the two models described above for the case when a single conductance quantum is observed experimentally. A statistical description based on a nearly free electron picture assumes that the constriction contains a single electronic channel. Because of the properties of the (random) connexions to the bulk electrodes, in most cases, the transmission of this channel is near one. The larger the number of channels in the external electrodes, the more likely it is to find a combination of the channels in the electrodes with a good matching to the channel in the constriction, explaining the observed clustering of conductances near h/e². Making a transformation to a basis in which these combinations are singled out, the model can be reduced to a one dimensional single channel problem, without loss of generality. The model, however, requires two barriers, at the two connexions of the weak link with the electrodes, as shown in fig. 1. On the other hand, a model based on atomic orbitals with nearest neighbor hybridization, in which the constraint narrows to a single atom, can be made equivalent, in the normal state, to a number of electronic channels of the order of the number of orbitals in one atom. Because of the small size of the constriction, the description of the transmission through each of these channels by a single barrier is highly plausible. Note, however, that the formation of the superconducting condensate can introduce changes in this picture at scales comparable to the gap.

In the following, we analyze the I-V characteristics of superconducting structures made up of a single channel with two barriers, which separate the constriction from the bulk electrodes. We can always hybridize the channels in the bulk electrodes (regions I and III in figure 1) in such a way that only one is coupled to the channel within the constriction. Thus, without loss of generality, the problem is reduced to that of a single channel interrupted by two barriers.
is the Fermi velocity, and \( k \) discussed later.

In the normal state, the system formed by the two barriers in series has an energy dependent transmission:

\[
T(\epsilon) = \frac{T_1 T_2}{1 + R_1 R_2 - 2 \sqrt{R_1 R_2} \cos (\phi_0 + 2f \frac{\epsilon}{\Delta})}
\]

where \( R_i = |t_i|^2 \) and \( T_i = |t_i|^2 \) are the reflection and transmission coefficients at each barrier.

The most general form of the wavefunctions at regions I, II and III, is:

\[
\Psi_I^s = \sum_{m,n} \left[ (a^{2m}_n A^m_n + J_0 \delta_{m0} \delta_{n0}) \right] e^{i k x} + B^m_n e^{-i k x}
\]

\[
\Psi^h = \sum_{m,n} \left[ A^m_n e^{i k x} + a^{2m}_n B^m_n e^{-i k x} \right] e^{-i(e+2neV_1+2neV_2)t}
\]

\[
\Psi_{I1}^R = \sum_{m,n} \left[ (a^{2m+1}_{n+1} E^m_n + F^m_n) e^{i k x} + (a^{2m+1}_{n+1} E^m_n + F^m_n) e^{-i k x} \right] e^{-i[(e+2n+1)eV_1+2neV_2]t}
\]

\[
\Psi_{I1}^I = \sum_{m,n} \left[ (E^m_{n-1} + a^{2m-1}_{n-1} E^m_{n-1}) e^{i k x} + (E^m_{n-1} + a^{2m-1}_{n-1} E^m_{n-1}) e^{-i k x} \right] e^{-i[(e+2n-1)eV_1+2neV_2]t}
\]

\[
\Psi_{II}^{R1} = \sum_{m,n} \left[ C^m_n e^{i k x} + a^{2m+1}_n D^m_n e^{-i k x} \right] e^{-i[(e+2n+1)eV_1+2neV_2]t}
\]

\[
\Psi_{II}^{I1} = \sum_{m,n} \left[ a^{2m}_n C^m_{n-1} e^{i k x} + D^{m-1}_n e^{-i k x} \right] e^{-i[(e+2n-1)eV_1+2neV_2]t}
\]

where \( V_1 \) and \( V_2 \) are the voltage drops at the two barriers, \( a^m_n(\epsilon) = a(\epsilon+2neV_1+2neV_2) \) is the Andreev reflection amplitude, and \( J_0 \) in the first equation gives the incoming current. The matching conditions lead to a set of matrix equations between the coefficients \( A, B, C, D, E, \tilde{E}, \tilde{F}, \) and \( \tilde{F} \) in the wavefunctions. It can be shown, after some algebra, that the only finite coefficients have \( m = n \). This implies that physical quantities depend on the total voltage drop, \( V_1 + V_2 \). This is a consequence of our neglect of inelastic scattering in region II. Finally, the coefficients in region II, \( E, \tilde{E}, \tilde{F} \) can be written in terms of the other four, leaving a set of equations formally equivalent to those of a single junction. They can be solved using recurrent fractions, as described in [35].

The main difference with the case of a single barrier is the energy dependence of the phase, parametrized by \( f \). Multiple Andreev scattering is determined by the transmission coefficient of the constriction at different energies. Hence, it is reasonable to expect that this energy dependence has a significant influence on the I-V characteristics below the gap energy.

The model has four adjustable parameters: the absolute values, \(|t_i|^2\), the phase between \( r_1 \) and \( r_2 \), which we label \( \phi_0 \), and \( f \) as defined above.

We use the scattering formalism presented in [35], which is equivalent to the Green’s function method formulated in [36] and used in the interpretation of experimental I-V curves. Each barrier is defined by a scattering matrix:

\[
S_i = \begin{pmatrix}
  r_i & t_i \\
  t_i & r_i^{\dagger}
\end{pmatrix}
\]

where \( r \) and \( t \) are complex numbers which satisfy \(|r|^2 + |t|^2 = 1\), and which are defined up to a global phase. In [36], we assume time reversal symmetry. The electronic wavefunctions at the channels in the electrodes and within the constriction, fig. [36], are described as plane waves, \( \Psi_k(x) \sim e^{i k x} \). The quasiparticles energies, in the normal state, are linearized around the Fermi level, \( \epsilon_k = \epsilon_F + v_F (k - k_F) \), where \( \epsilon_F \) is the Fermi energy, \( v_F \) is the Fermi velocity, and \( k_F \) is the Fermi wavevector. Each wavefunction has different phases at the two barriers. The overall phase shift includes a contribution from the region described in terms of perfect channels, and a contribution from the matching zones, described phenomenologically by the scattering matrices. The phase shift can be written as an energy independent part plus an energy dependent contribution, which we parametrize as:

\[
\phi(\epsilon) = f \epsilon - \epsilon_F \frac{\Delta}{h}
\]

where \( f \) is dimensionless, and \( \Delta \) is the superconducting gap. If the transmission through the constraint is ballistic, we have \( f = \frac{\Delta}{h v_F} \), where \( L \) is the length of the region between the barriers. A more general situation is discussed later.
In fig. 2, we show the best fittings that we obtain to the I-V characteristics analyzed in (34) in terms of different channels in parallel. The method of minimization of the mean square deviations that we use leads to more than one possible fitting of similar quality. The parameter $f$ is 0.08 for the upper curve (which corresponds to a two channel model in (34)) and 0.1 for the lower curve (which corresponds to a three channel model in (34)).

Another quantity which has a non linear dependence on the transmission, and which can be used to elucidate the detailed structure of the constraint, is the critical current. In fig. 3 we show the dependence of the Josephson current (38) on the superconducting phase between the electrodes for the two cases analyzed in fig. (2) and for a single channel and one barrier of the same normal state conductance. The maximum value gives the critical current of the junction. Our results deviate from the single channel one barrier case in the opposite direction to those obtained by combining different channels.

In order to relate $f$ to the structure of the constraint, we assume that the motion of the electrons in the contact zones is diffusive, with a mean free path, $l$. The dependence of the phase shift on distance and frequency goes as $\frac{\omega}{D}$, where $D \approx \frac{v_F}{l^3}$ is the diffusion coefficient. Replacing $\omega$ by $\Delta$, we obtain:

$$f \sim \frac{\Delta L^2}{\hbar v_F l^2} \sim \frac{L^2}{\xi_0 l}$$  \hspace{1cm} (5)

where $L$ is the length of the constriction, and $\xi_0$ is the coherence length at zero temperature. Taking $\xi_0 \sim 10^4 \text{Å}$ for Al, the values of $f$ that we obtain, $\sim 0.1$, suggest values of the order of $L \sim 300 \text{ Å}$ and $l \sim 100 \text{ Å}$. These numbers are consistent with experimental observations (39).

The enhancement of the Andreev reflections that we find in a double barrier geometry is similar to the results obtained for transport through a single level between superconducting electrodes (40).

In summary, we find that existing experiments cannot rule out a description of many of the weak links which show conductance quantization in terms of a small number of channels (one for each quantum) randomly coupled to larger systems described by a much higher number of channels. This description is consistent with the observed statistical distribution of the normal state conductance. Our fitting of experimental results require constrictions of typical dimensions $L \sim 300 \text{ Å}$, and strong disorder, with mean free paths $l \sim 100 \text{ Å}$. The size of the constriction, and the existence of strong disorder, are compatible with existing experiments.
The model analyzed here, however, needs not apply to all observed cases, as it only attempts to describe an average situation. When the constriction size is of the order of a single atom, it is plausible conducting evanescent waves (in our language) play some role. If their contribution to the conductance is a significant fraction of the total value, a description based on extended wavefunctions is almost indistinguishable from one based on localized atomic orbitals. On the other hand, the existence of well defined conductance steps near integer multiples of $2/e^2$ seems to us more consistent with a dominance of situations with almost fully conducting channels within the constriction.

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