Andreev scattering in nanoscopic junctions in a magnetic field

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Abstract. – We report on the measurement of multiple Andreev resonances at atomic size point contacts between two superconducting nanostructures of Pb under magnetic fields higher than the bulk critical field, where superconductivity is restricted to a mesoscopic region near the contact. The small number of conduction channels in this type of contacts permits a quantitative comparison with theory through the whole field range. We discuss in detail the physical properties of our structure, in which the normal bulk electrodes induce a proximity effect into the mesoscopic superconducting part.

It is well known that it is possible to fabricate atomic size contacts between metallic electrodes by means of the mechanically controllable break junction technique or the scanning tunneling microscope (STM) \[1,2\]. Indeed, by repeatedly indenting the tip into the sample of an STM a stationary state is achieved in which a connecting neck between the electrodes is formed \[3,4\]. This neck elongates and contracts during the repeated indentation following a well-defined pattern of elastic and plastic steps, which has been neatly measured in a combined STM-AFM experiment where conductance and forces could be recorded simultaneously \[5\].

A reasonable knowledge of the geometry of the neck, which can be varied in a well-controlled way, is obtained through a simultaneous measurement of the conductance during the fabrication process \[4\]. The STM serves at the same time as a fabrication tool and as an experimental probe of a very singular atomic size nanostructure \[4,5\]. The final form of these structures, which are successfully fabricated \[4,6,7\], is a long connecting neck joined on its ends to the bulk electrodes whose radius decreases in a smooth way towards a central constriction, which can consist of a single atom (\(i.e.\) the last contact before completely separating two electrodes, see \[2,8–10\]). It is important to realize that the STM permits us to
change the overall form of the neck at mesoscopic length scales (hundreds or thousands of Å) by changing the position on the surface where we do the repeated indentation process. We can also, without varying the overall form of a given neck, completely change the atomic configuration around the single-atom point contact by gently moving the tip at atomic length scales (tens of Å). In the following we will use the word neck to refer to the mesoscopic geometry of the sample and the word atomic contact to refer to the narrowest cross-section, which in the results presented here consists only of one atom.

Recently new possibilities of atomic size contacts have led to progress on the understanding of some phenomena occurring at a nanoscopic level. The authors of refs. [8, 9] proposed that information about the number and transparency of the conduction channels through a single atom could be obtained by analyzing the effect of Multiple Andreev Reflection (MAR) processes on the $I$-$V$ curves of superconducting atomic point contacts. It has been shown during the last years that lead (Pb) is a good material to create this kind of small dimensions systems having the additional advantage of being a superconductor below $T_c = 7.16$ K [3].

In this work we study the magnetic field dependence of the $I$-$V$ characteristics of superconducting single-atom point contacts. It is well known that superconductors of reduced dimensions such as thin films or granular samples remain superconducting well above the bulk critical field $H_c$ [11]. As the magnetic field penetration depth of lead is about 390 Å for a bulky sample, it is feasible to build connecting necks with smaller lateral dimensions by repeated indentation [4, 7]. We find indeed that sufficiently long and narrow necks show superconducting features up to fields as large as 20 times $H_c$ (= 0.05 T at 1.5 K) [12]. For fields larger than $H_c$, superconductivity is restricted to a mesoscopic region near the contact. We report here on the measurement and detailed analysis of the Andreev resonances that appear in single-atom contacts, under magnetic fields. We obtain quantitative comparison with theory, by precisely modeling the changes induced by the magnetic field on the neck. We characterize the superconducting neck which is intimately embedded in normal electrodes for $H > H_c$.

We use a stable STM setup with a tip and a sample of the same material (Pb) which is brought from the tunneling into the contact regime by cutting the feedback loop. The $I$-$V$ curves were taken at 1.5 K using a standard four-wire technique [8, 9]. Great care was taken to shield electrically the whole setup as RF noise is known to smear the subgap resonances in small contacts. The maximal elongation of the piezotube, which is 1600 Å, limits the overall length of the necks. The experiment is done making a large number of atomic size contacts at each magnetic field without varying the overall form of the neck in a given field sweep (up to fields of 2 T). In the figures of this paper, we present one typical case of a neck having a critical field of about 20 times the bulk critical field of lead with a magnetic field applied parallel to the long axis.

Figure 1a shows a representative choice of measured $I$-$V$ curves of several single-atom contacts at zero field. The curves show a large variety of behaviours. By changing the atomic rearrangement, the conductance $\sigma$ of a single-atom contact of Pb varies between 1 and $3\sigma_0$ (the quantum of conductance $\sigma_0 = 2e^2/h$) [10]. The curves are strongly nonlinear for $V \leq 2\Delta$ with singularities, usually called subharmonic structure, at $V = 2\Delta/l$, with $l$ an integer number. For voltages $V \gg 2\Delta$ curves are linear with $I = I_{\text{exc}} + \sigma V$ with $I_{\text{exc}}$ the excess current. These features are due to Multiple Andreev Reflection processes [11]. Contacts with equal or very similar conductances have very different $I$-$V$ curves. As discussed in refs. [8, 9, 13], we also find that it is possible, using the theoretical calculations [14, 15], to fit every $I$-$V$ curve. For that it is, as in previous references [8, 9], assumed that one atom can sustain several conducting modes or channels and separate the contributions from each channel $\sigma = \sigma_0 \sum_{n=1}^{N} T_n$, with $N$
Fig. 1 – $I$-$V$ characteristics of atomic sized contacts in the presence of a magnetic field taken at 1.5 K. From a to d: $\Delta = \Delta_0$, 0.97$\Delta_0$, 0.94$\Delta_0$, 0.88$\Delta_0$ and $\Delta_0 = 1.35$ meV (as measured). $I$ is normalized to $\Delta$ and $\sigma$, the conductance above $2\Delta$ in units of $\sigma_0$. Not all experimental points are plotted in order to show more clearly the fits (full lines) using the model explained in the text. The parameters in the lower right corner of each figure are the transmissions through the different channels used to fit the experimental data. Each line of numbers corresponds to one curve, from top to bottom. $\Gamma$ is the pair-breaking parameter (defined in the text).

being the number of conduction channels through the contact and $T_n \leq 1$ the transmission of a given channel. $N$ depends on the element studied and is 3 in the case of Pb (see [9,16] for data in other superconductors) and $\{T_n\}$ depends on the atomic arrangement of the neighbors of the contacting atom, and is therefore different for each single-atom contact. Exact values for $N$ and $\{T_n\}$ are indeed obtained which give very good fittings. Due to the strong nonlinearity of the curves, variations as small as 1% in the set $\{T_n\}$ give a significant deviation from the experiments.

Figures 1b-d show a characteristic set of curves measured under magnetic field. As the field is increased the subharmonic structure is smoothed. To explain the data under field we first analyze the influence of the magnetic field introducing the pair-breaking effect in the standard procedure [8], as formulated in a wave function representation [13, 15, 17–19]. It was shown in [17] that pair-breaking effects can be incorporated by modifying the Andreev reflection amplitude, $a(\omega) = u(\omega) - \sqrt{u^2(\omega) - 1}$, where $u(\omega)$ satisfies [20]

$$\frac{\omega}{\Delta} = u \left( 1 - \Gamma \frac{1}{\sqrt{1 - u^2}} \right),$$

where $\Gamma = h/(\Delta \tau_{pb})$, $\tau_{pb}$ is the pair-breaking time and $\Delta$ is the self-consistent superconducting order parameter, including the pair-breaking effects. For $\Gamma < 1$, there is a gap in the spectrum of magnitude $E_g = \Delta (1 - \Gamma^2/3)^{3/2}$. In the dirty limit (mean free path $\ell < \xi$) and assuming a uniform order parameter, this expression is generally valid, irrespective of the origin of the pair-breaking mechanism [20]. The value of $\Gamma$ used in the fittings was assumed to be the same
for all channels and all $I$-$V$ curves at a given applied field.

The lines in fig. 1b, c and d show the fittings. The quality of the fittings does not change as a function of the field, provided that $\Gamma$ is introduced. Even if the subharmonic gap structure is smoothed under field, the strongly nonlinear form of the curves for $V < 2\Delta$ remains, so that each contact can be well characterized in terms of $N$ and $\{T_n\}$ up to the highest measured fields. For instance, changes larger than 5% in $\{T_n\}$ (in fig. 1d) result in a clear deviation between theory and experiment. Therefore, we conclude that the magnetic field does not change the essential properties of the contact, in the sense that when the field is applied no conduction channel is closed nor a new channel opens ($N = 3$). In order to obtain an additional check of this point, we have done small sweeps of 300 G at different fields and observed no changes in the $I$-$V$ curve, other than the pair breaking, modeled by $\Gamma$. This is not surprising, as the flux going through the contact, even at fields of several teslas, is much too small to produce changes in the electronic transport in the neck or in the orbital structure of the contacting atom.

The introduction of $\Gamma$ means that the superconducting properties of the neck clearly change and seem to be correctly modeled by this approach taking Maki’s pair-breaking parameter [20]. Changes larger than 0.01 in the value of $\Gamma$ for a given contact result in a clear deviation from experiment, which cannot be recovered by changing $\{T_n\}$. It is important to realize that the fitting parameters $\{T_n, \Gamma\}$ are well defined, the values we give are the only ones which give a good fitting to the experimental curve. In order to gain further insight in our system, we try to relate in the following the absolute values of $\Gamma$ to the geometry of our system. Indeed, for an infinite cylindrical wire, the pair-breaking time is directly related to the radius of the cylinder $R$ through [20]

$$\frac{\hbar}{\Delta_0 \tau_{pb}} = \frac{\xi^2 R^2}{3 l_H^4},$$

(2)

where $\xi$ is the coherence length and $l_H$ the magnetic length, given by $l_H = 256 \, \text{Å}/\sqrt{H}$, where $H$ is in teslas. If we take $\xi \approx R$, and for the radius of the cylinder the mean radius $R \leq 250 \, \text{Å}$ of a typical neck (fig. 1, see also [4, 7]), we obtain values of $\Gamma$ 15–30 times smaller than the ones needed to fit our curves. Moreover if, assuming the dependence of the pair-breaking time on the field given by (2), we extrapolate the values of the pair-breaking parameter obtained to large fields, the superconductivity should disappear at fields of the order of 0.35 T, while in the experiment it remains up to much larger fields. It is therefore impossible to give a physical meaning to the values of $\Gamma$ using such a simple model to describe the geometry of our system, although we obtain a good fit to the $I$-$V$ curves under a field.

Therefore, we relax the assumption of an infinite neck of constant radius. To do so, we use Usadel’s equations [21–24] and analyze the superconducting properties of a neck of varying radius, assuming, as before, that $l < \xi$. We parametrize the Green’s functions in terms of an angle variable, $\theta(\vec{r}, E)$, where $\vec{r}$ is the position vector and $E$ is the energy measured from the chemical potential [25]. In the present case, we have $g = \cos(\theta)$ and $f = \sin(\theta)$, and $g$ and $f$ are the normal and anomalous Green’s functions. Setting $\hbar = 1$, Usadel’s equations can be written as

$$\frac{D}{2} \nabla^2 \theta + i E \sin(\theta) + |\Delta| \cos(\theta) - 2 e^2 D |\vec{A}|^2 \cos(\theta) \sin(\theta) = 0.$$  

(3)

We use cylindrical coordinates $(r, \phi, x)$ being the neck parallel to the $x$-axis. $\vec{A} = (Hr \vec{u}_\phi)/2$ is the vector potential. We only consider the pair-breaking effects due to the applied field, and neglect other inelastic scattering processes. The geometry of the contact is described by the function $R(x)$, which gives the local radius of the neck (see below). Finally, we assume that the magnetic field is unscreened and neglect the radial dependence of the quantities of interest.
Fig. 2 – Panel a shows the superconducting order parameter as a function of distance, for different applied fields corresponding to the geometry described in the text. The contact region is located at $x/\xi_0 = 0$. The neck (shown in the inset) is joined to the electrodes at $x/\xi_0 = 2.6$. The magnetic field is applied along the long axis of the cones. The density of states at the contact is plotted in panel b. The inset shows the shape of the density of states corresponding to the model in which the magnetic field is introduced through the single parameter $\Gamma$ [20, 26].

Then, $\mathbf{A}^2$ can be replaced by its average, $\langle \mathbf{A}^2 \rangle (x) = \frac{\hbar^2 R(x)^2}{12}$. Within this approximation, the field enters in eq. (3) as an effective, position-dependent, pair-breaking time. The knowledge of the energy- and position-dependent Green’s functions of the system allows us to characterize the zone where the crossover from the normal to the superconducting properties takes place.

Figure 2a shows the superconducting order parameter, for different fields, as a function of the position for a typical neck. The neck (see inset of fig. 2a) is modeled by the simplest geometry consistent with the experimental information available, two truncated cones each of length $L$, with an opening angle of $\alpha$, joined by their vertices and attached to the bulk electrodes (see also [4]; in the figures we take $\xi_0 = 325$ Å, $L = 850$ Å = $2.6\xi_0$ and $\alpha = 45^\circ$, these values give a good fit to the experimental curves, as discussed further on). There is a smooth transition to the normal state as the radius of the neck increases. Even at the central region, the gap is significantly rounded. This is also observed in the calculated density of states at the center shown in fig. 2b for different values of the field. For a neck with this geometry, superconductivity survives up to fields much larger than in the previous description, compatible with the experimental results. It is worth remarking that these results depend on the geometry of the neck, being $\xi_0$ the characteristic length scale, and are insensitive to the details of the contact at atomic scales.

In the inset of fig. 2b the density of states corresponding to the model used to make the fits in fig. 1 is plotted for different values of $\Gamma$ [20, 26]. The form of the density of states differ between both approaches, the density of states at the Fermi level $N(E = 0)$ from Usadel equations being finite even at low fields. However, for the values of the fields used in the experiment, the amplitude of Andreev reflections (given by $i \tan[\theta(x = 0, E)/2]$) obtained in both models does not differ too much and give quite similar $I$-$V$ curves. We have recalculated $I$-$V$ curves of fig. 1 using the Usadel equations. The results are shown in fig. 3. As the overall shape of the neck is not varied in the experiment, we use the same geometry and coherence length to explain all the curves for all the fields. We are able to
fit all the curves for the geometry described above, as shown in fig. 3. We have used the
same transmission coefficients as in fig. 1, and obtained similar numerical accuracy. Thus, by
comparing the two schemes, we can separate the effects of the nanoscopic contact, contained
in the set of transmission coefficients, \( \{ T_n \} \), from the effects due to the neck geometry and the
NS interface at the electrodes. The pair-breaking parameter \( \Gamma \), used in the fittings in fig. 1,
describes, approximately, the details of the geometry and the interface between the normal and
superconducting regions, which are better captured in the full solution of Usadel’s equations.
Because of this, \( \Gamma \) cannot be related to the properties of a neck of constant width.

However, we do not always find a one-to-one correspondence between both approaches in
the quality of the fits. We have found significant deviations between the two methods in the
case of a sufficiently short and wide neck with respect to \( \xi \), or also at high fields, near the
complete destruction of superconductivity. In both situations, the normal-superconducting
interface moves very close to the contact and the amplitudes of Andreev reflections obtained
from both models are different enough to obtain different \( I-V \) characteristics. Then, a descrip-
tion of the superconducting features in terms of parameters valid for a homogeneous system
is no longer applicable [27].

Note that we could follow and fit precisely the predicted influence of pair breaking on
the structures associated with multiple Andreev reflections. Former experimental realiza-
tions (see [11]) involve experimental setups having a large number of conduction channels and
cannot be modeled precisely. In order to further experimentally verify the conclusions of this
paper, we have repeated the measurement in a large number of necks, with slightly different
geometries and the field applied parallel or perpendicular to the long axis of the neck, always
finding the same results, i.e. that the characteristics of the single-atom point contact do not
vary with field, and that one needs to go beyond the conventional description of pair breaking
and use the model presented here to understand the values needed to fit the curves.

In conclusion we have measured and analyzed the multiple Andreev scattering resonances
of atomic sized Pb contacts in the presence of a magnetic field greater than the bulk critical
field. In this regime, superconductivity is restricted to a small neck of mesoscopic dimensions.
We are able to build and control in situ with our STM structures which are a unique example
of weak links of dimensions variable from atomic to mesoscopic length scales. We present a
quantitative comparison of experiment and theory of pair-breaking effects on multiple Andreev resonances, and discuss the main superconducting features of the system.

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