Impurity states in mesoscopic SNS junctions with a point defect

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Abstract. We study theoretically localized states in a clean three-dimensional SNS junction, containing one point defect (impurity) located in the normal layer. We find that the defect induces two quasibound states in a short junction, corresponding to different spin projections. The energies of these states coincide for a nonmagnetic defect and are generally different for a magnetic defect. The spatial structures of the impurity states resemble the structures of Shiba states in a bulk superconductor. We also consider the case when the impurity is located close to a flat edge of the junction. We find mesoscopic fluctuations of the energies of the quasibound states as a function of the distance between the impurity and the edge.

1. Introduction

The phenomenon of sample-to-sample fluctuations of transport characteristics is one of the key problems in modern mesoscopic physics and nanotechnology. A number of fascinating results in this field are related, for example, to universal conductance fluctuations in normal metal systems (see [1] for a review) and critical current fluctuations in short SNS junctions [2] and SFS junctions [3, 4]. Later on, similar problems have been analyzed within the nonlinear sigma model in longer SNS junctions: the fluctuating density of states [5] and Josephson current [6] have been determined. Most of these studies concentrate on the calculation of the root-mean-square deviation of the current from its average value. Such calculations can be compared with experiment by averaging over a large number of samples. For a given sample, it might be important to understand how a given realization of disorder, e.g. several impurities affect its characteristics. Individual impurities can be nicely observed by the STM technique [7] (see [8] for a recent study of magnetic impurities on a two-dimensional superconductor). It is the goal of the present study to analyze the electronic structure of a single impurity atom in a short Josephson junction with a large number of transport modes. The formation of localized impurity states in a bulk superconductor has been previously stated for a number of systems, including magnetic impurities [9, 10, 11] or nonmagnetic defects inside an unconventional superconductor [12]. In this work we use a more general approach which allows to take into account the inhomogeneity of the superconducting order parameter to find the localized impurity states as well as the whole density of states in the presence of a nonmagnetic or magnetic point defect. Our approach is applicable for arbitrary impurity positions and strengths, providing the basis for further studies of quasiparticle interference patterns in random impurity arrays.
2. Infinite SNS junction with a point defect

We will start by considering an infinite SNS junction with a nonmagnetic point defect located in the normal layer, as depicted in Fig. 1a. We assume a step-like order parameter profile in the junction: the gap $\Delta(\mathbf{r})$ is equal to $\Delta_j e^{i\varphi}$ in the left superconducting bank and $\Delta_j e^{i\varphi}$ in the right superconducting bank, where $\Delta_j = \text{const}$ and $\varphi = \text{const}$. Such a model is justified, for example, for junctions of the constriction type [13], where $\Delta(\mathbf{r})$ may vary strongly on a scale much smaller than the superconducting coherence length $\xi$. In the normal layer we put $\Delta = 0$.

![Figure 1. In\(\text{finite (a) and semi-in\(\text{finite (b) SNS junction with a point defect.}

We will analyze the spectral characteristics of subgap states in the junction. These characteristics can be extracted from the $2 \times 2$ matrix retarded Green function $G_E(\mathbf{r}, \mathbf{r}')$, which satisfies the Gor’kov equation [14]

$$\begin{align*}
\hat{0}
& \left[ H_0(\mathbf{r}) + U(\mathbf{r} - \mathbf{r}_1) \right] - \hat{\tau}_z (E + ie^+) + \\
& \begin{pmatrix}
0 & -\Delta(\mathbf{r}) \\
\Delta^*(\mathbf{r}) & 0
\end{pmatrix}
\right] G_E(\mathbf{r}, \mathbf{r}') = \hat{0}\delta(\mathbf{r} - \mathbf{r}').
\end{align*}$$

Here, $\hat{0}$ and $\hat{\tau}_z$ are a unit matrix and Pauli matrix in Nambu space, respectively, $H_0(\mathbf{r})$ is the normal-state Hamiltonian of a pure system, $U(\mathbf{r})$ is the electric potential of the impurity, the vector $\mathbf{r}_1$ indicates the position of the impurity, $E$ is the energy and $e^+$ is an infinitely small positive quantity. For our infinite system, we will use the simple normal-state Hamiltonian

$$H_0(\mathbf{r}) = -\hbar^2 \nabla^2 \over 2m - \mu, \quad (2)$$

where $m$ is the electron mass, $\mu = \hbar^2 k_F^2 / (2m)$ is the chemical potential, and $k_F$ is the Fermi wave number. Now we will use the fact that the defect is small: specifically, we mean that the range of the potential $U(\mathbf{r})$ is much smaller than $k_F^{-1}$. Then the impurity is essentially an isotropic point scatterer, which is completely characterized by an energy dependent scattering phase $\alpha(E)$. This means that the wave function of an electron will have the following form in the vicinity of the defect [15]:

$$\psi(\mathbf{r}) = \psi_{in}(\mathbf{r}) + \frac{\psi_{in}(\mathbf{r}_1)e^{ik(|\mathbf{r} - \mathbf{r}_1|) + i\alpha}}{k|\mathbf{r} - \mathbf{r}_1|} \sin \alpha, \quad (3)$$

where $\psi_{in}(\mathbf{r})$ is a regular function, and $k$ is the energy dependent wave number. Equation (3) means that a point defect in the Schrödinger or Gor’kov equations can be incorporated as an effective boundary condition at the point $\mathbf{r} = \mathbf{r}_1$ [16]. This observation allows to solve Eq. (1) in terms of the Green function $\hat{G}_E^{(0)}(\mathbf{r}, \mathbf{r}')$ of the system without the defect:

$$\hat{G}_E^{(0)}(\mathbf{r}, \mathbf{r}') = \begin{pmatrix}
G_E^{(0)}(\mathbf{r}, \mathbf{r}') & F_E^{(0)}(\mathbf{r}, \mathbf{r}') \\
-F_E^{(0)*}(\mathbf{r}, \mathbf{r}') & \hat{G}_E^{(0)}(\mathbf{r}, \mathbf{r}')
\end{pmatrix}.$$
Taking \( E \ll |\Delta| \) and assuming that \( \alpha \approx \text{const} \) for such energies, we obtain the following solution of Eq. (1):

\[
\hat{G}_E(r, r') = \hat{G}_E^{(0)}(r, r') + \frac{\hat{G}_E^{(1)}(r, r', r)}{\mathcal{D}(E, r_1)},
\]

where

\[
\mathcal{D}(E, r_1) = \left[ \frac{mk_F \cot \alpha}{2\pi \hbar^2} - G_{ER}^{(0)}(r_1, r_1) \right] \left[ \frac{mk_F \cot \alpha}{2\pi \hbar^2} - G_{-ER}^{(0)}(r_1, r_1) \right] + F_{E}^{(0)}(r_1, r_1) F_{-E}^{(0)*}(r_1, r_1),
\]

and \( \hat{G}_E^{(1)}(r, r', r) \) is a combination of the components of \( \hat{G}_E^{(0)}(r, r') \) which has only poles coinciding with those of \( \hat{G}_E^{(0)}(r, r') \). Additional poles of the Green function appear at energies where the denominator \( \mathcal{D}(E, r_1) \) vanishes. These are the energies of impurity-induced bound states. We will now analyze such states in our SNS junction. Generally speaking, the matrix \( \hat{G}_E^{(0)}(r, r') \) can be determined for a junction with arbitrary length \( L \), however, the most interesting situation occurs in short junctions with \( L \ll \xi \). We have then

\[
G_{ER}^{(0)}(r_1, r_1) \approx \frac{mk_F}{4\pi \hbar^2} \left[ \cot \left( \gamma(E) + \frac{\varphi}{2} \right) + \cot \left( \gamma(E) - \frac{\varphi}{2} \right) \right],
\]

\[
F_{E}^{(0)}(r_1, r_1) \approx \frac{mk_F}{4\pi \hbar^2} \left[ \sin^{-1} \left( \gamma(E) + \frac{\varphi}{2} \right) + \sin^{-1} \left( \gamma(E) - \frac{\varphi}{2} \right) \right],
\]

where

\[
\gamma(E) = \arccos \left( \frac{E}{\Delta} \right).
\]

One finds then that \( \mathcal{D}(E, r_1) \) vanishes at an energy

\[
E_A = |\Delta| \sqrt{1 - \sin^2 \frac{\varphi}{2} \cos^2 \alpha - iE'_A(\alpha, \varphi, r_1)},
\]

where \( E'_A \sim |\Delta| L/\xi \). This corresponds to two spin-degenerate localized states. The presence of an imaginary part of the energy means that the impurity states are in fact resonances with a finite lifetime. This is easy to understand: a quasiparticle localized at the impurity will “leak” to infinity along the normal layer (note that in [2] in a short disordered SNS junction no quasibound states have been found, because a finite system has been considered). The quasibound states in the SNS junction are somewhat similar to Yu-Shiba-Rusinov states [9, 10, 11] in bulk superconductors: their spatial structure is roughly a bubble with a radius of the order of \( \xi(1 - E^2/|\Delta|^2)^{-1/2} \).

Equation (11) has an interesting interpretation in view of the theory of Beenakker [2] applicable to short SNS junction. It means that the point impurity blocks one transmission channel (per spin projection) in the normal layer, reducing its transparency from unity to \( \tau = \cos^2 \alpha \). All other channels remain completely transparent.

The theory developed above can be generalized for a magnetic impurity. In this case, a spin quantization axis can be chosen such that electrons with “spin up” and “spin down” will be scattered by the defect with phases \( \alpha_+ \) and \( \alpha_- \), respectively. The real parts of the energies of impurity states with spin projection \( \sigma \) are then given by

\[
\frac{E_\sigma}{|\Delta|} \approx \sigma \sin \beta \sqrt{\cos \alpha_+ \cos \alpha_- \sin^2 \frac{\varphi}{2} + \sin^2 \beta \pm \cos \beta \sqrt{\cos^2 \beta - \cos \alpha_+ \cos \alpha_- \sin^2 \frac{\varphi}{2}}},
\]

where \( \sigma = \pm 1 \), and \( \beta = (\alpha_+ - \alpha_-)/2 \). Generally, Eq. (12) yields two negative and two positive values of \( E_\sigma \), the latter two corresponding to the true energies of the impurity states. Depending on relations between \( \alpha_+ \), \( \alpha_- \) and \( \varphi \), one may have two quasibound states with either the same spin or opposite spins. Some \( E_\sigma \) vs. \( \varphi \) graphs are shown in Fig. 2.
3. Semi-infinite SNS junction with a point defect

Real Josephson junction have a finite size, thus it is important to understand how boundaries of the system influence the impurity states. In this section we consider a semi-infinite SNS junction, as shown in Fig. 1b. Here, the half-space $y < 0$ is occupied by the junction, and the half-space $y > 0$ is occupied by vacuum. On the edge of the junction we impose the boundary condition

$$\hat{G}(r, r') \bigg|_{y=0} = 0.$$  

Then, the Green function $G^{(0)}(r, r')$ can be obtained using the image method. We find then that the energies of the impurity states are still given by Eqs. (11) and (12) with the scattering phases replaced by their effective values $\alpha_{\text{eff}}$ defined as

$$\cot \alpha_{\text{eff}} = \frac{\cot \alpha + \frac{\cos(2k_F h)}{2k_F h}}{1 - \frac{\sin(2k_F h)}{2k_F h}},$$  

where $h$ is the distance between the impurity and the edge of the junction. Remarkably, the phase $\alpha_{\text{eff}}$ is an oscillating function of $h$, and hence the energies of the impurity states also oscillate when $h$ is changed. This is a simple illustration of mesoscopic fluctuations in a system with low disorder. Note that the oscillations decay on a scale $h \sim k_F$, so that even if the distance $h$ is much smaller than the spatial extent of the impurity states $(k_F^{-1} \ll h \ll \xi)$, their energies may be very weakly affected by the surface of the junction. Some typical graphs of the impurity state energies vs. $h$ dependencies are shown in Fig. 3.

4. Conclusion

We have analyzed the localized states induced by a point impurity in a short SNS junction. The impurity generally supports two quasibound states, which may have the same spin or opposite spins (in the case of a magnetic impurity). If the defect is located close to the edge of the junction, the energies of the localized states become sample-specific: they exhibit mesoscopic fluctuations when the distance between the impurity and the sample edge is changed.

There are several observable effects related to the impurity states. First, since the defect blocks a transport channel in the normal layer, it reduces the critical current of the junction. For example, at low temperatures a unitary impurity with $\alpha \approx \pi/2$ should reduce the critical current by a value of the order of $e|\Delta|/h$ (see [2]), where $e$ is the elementary charge. Another way to observe the impurity states is by using the STM technique, which allows to measure both the energies and the spatial structures of the localized states.

Figure 2. Energies of “spin-up” ($\uparrow$) and “spin-down” ($\downarrow$) quasilocalized states at a magnetic impurity.
Figure 3. Dependencies of the impurity state energy $E$ on the distance $h$ between a nonmagnetic impurity and the surface of the SNS junction for $\varphi = \pi$. The scattering phases $\alpha$ are positive in graph (a) and negative in graph (b).

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