Yu-Shiba-Rusinov bands in superconductors in contact with a magnetic insulator

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Abstract

Superconductor-Ferromagnet (SF) heterostructures are of interest due to numerous phenomena related to the spin-dependent interaction of Cooper pairs with the magnetization. Here we address the effects of a magnetic insulator on the density of states of a superconductor based on a recently developed boundary condition for strongly spin-dependent interfaces. We show that the boundary to a magnetic insulator has a similar effect like the presence of magnetic impurities. In particular we find that the impurity effects of strongly scattering localized spins leading to the formation of Shiba bands can be mapped onto the boundary problem.

Keywords:

Over the last two decades a tremendous progress in creating and controlling heterostructures consisting of superconductors and ferromagnets have been achieved both on an experimental and a theoretical level. \cite{1, 2, 3, 4, 5, 6}. The progress has been reviewed in \cite{7, 8}. More recently, the experimental focus has shifted toward magnetic insulators, offering certain advantages like the absence of low-energy electronic excitations responsible for the loss of superconducting coherence, and efficient spin filtering \cite{9, 10, 11}. In this way, a long-range spin transport was demonstrated \cite{12, 13} or extremely large thermoelectric transport
Figure 1: Sketch of a superconducting layer in contact with a magnetic insulator. Some of the surface spins might point in the opposite direction.

At low temperatures \[14, 15\]. Recently tunneling spectroscopy was reported \[16\]. On the theoretical side, it has been shown that the proximity to magnetic insulator leads to a suppression of the critical temperature \[17\] using spin-dependent boundary conditions for the quasiclassical Green functions. On the basis of a diffusive description, the induced exchange splitting was used to suggest an absolute spin-valve effect \[18\]. The boundary conditions have been developed further \[19, 20\] into the present most general form \[21\].

The quasiclassical problem of the density of states in a superconductor close to a magnetic insulator as shown in Fig. 1 is readily formulated in terms of the quantum circuit theory. We define the spin-dependent Green functions for spin direction \(\sigma\) in Nambu space via \(\hat{g}_\sigma = g_\sigma \hat{\tau}_3 + f_\sigma i \hat{\tau}_2\) with ubiquitous normalization condition \(g^2_\sigma + f^2_\sigma = 1\). The boundary condition for strongly spin-dependent scattering has been derived in \[21, 20\] and for the present case takes the form

\[-i(E + \sigma \mu_B B) f_\sigma - \Delta g_\sigma + i\sigma f_\sigma \epsilon \left( \frac{\sin(\phi/2)}{\cos(\phi/2) - i\sigma g_\sigma \sin(\phi/2)} \right) = 0. \tag{1}\]

Here \(\mu_B B\) is the Zeeman energy due to an external magnetic field, \(\Delta\) the self-consistent pair potential, \(\epsilon = r_S E_{Th} G_Q / G\) an parameter determining the effective influence of the interface on the superconductor with the Thouless energy \(E_{Th}\), the conductance per area \(G\) of the superconducting film in perpendicular direction, the quantum conductance \(G_Q = 2e^2/h\) and the fraction \(r_S\) of spin-active scattering channels at the interface. \(\langle \cdot \cdot \cdot \rangle\) denotes a suitable average over the spin-dependent interfacial phase shifts.
This equation is solved numerically and some results are shown in Fig. 2. Figs. 2(a) and (b) illustrate two limiting cases with a single spin-mixing angle. For weak spin mixing, Fig. 2(a), spin-active scattering is equivalent to a Zeeman field, as has been noted earlier by expanding the boundary conditions in orders of $\phi$ [19]. For strong spin mixing, Fig. 2(b), energy bands develop within the energy gap of the superconductor. These bands are fully spin polarized, in analogy to the Andreev bound state in a single-channel superconductor-ferromagnet point contact [22, 23, 24]. The subgap energy bands are remarkably similar to the well-known Shiba bands formed by bound states at spinfull impurities [25, 26, 27], studied experimentally in [28, 29, 30]. For ferromagnetically aligned impurities,
the Shiba bands are also predicted to be spin polarized \[31\]. This raises the question how spin-active scattering at interfaces in the diffusive limit is linked to spin-dependent scattering at randomly distributed magnetic impurities. We therefore can try to map the equations for the DOS in a superconductor in contact with a strong ferromagnetic insulator to the known behavior of strong magnetic impurity bands (strong means here in the presence of Shiba states). The old problem has been treated in \[32\] extending the work by Shiba \[25, 26, 27\]. Shiba has shown that a strong magnetic impurity in a superconductor leads to the formation of a bound state with energy

\[ E_B = \Delta \frac{1 - \gamma^2}{1 + \gamma^2} \equiv \Delta \varepsilon_B \tag{2} \]

where \( \Delta \) is the superconducting gap energy and scattering parameter \( \gamma^2 = \pi^2 S(S+1)J^2 N_0^2 \). Zittartz and coworkers have shown that the equation for the Green function can be cast in the form

\[ \frac{\omega}{\Delta} = u \left( 1 - i \frac{\Gamma}{\Delta} \frac{\sqrt{u^2 - 1}}{u^2 - \varepsilon_B^2} \right) \tag{3} \]

Here \( \Gamma \) is a parameter related to the spin-flip scattering rate and depends e.g. on the impurity concentration. The density of states follows from \( N(E) = \text{Re}[u/\sqrt{1-u^2}] \) and some resulting forms of the DOS are found in \[32\].

To compare this with our result using the spin-mixing angle we note that spin mixing leads not only to pair breaking, but simultaneously adds an exchange energy shift. To overcome this, let us assume that we have the same number of positive and negative phase shifts. This corresponds roughly to a random orientation of the impurity spin, which is the same assumption as in \[32\]. Hence, we obtain the following equation from \[11\]

\[ 0 = i \omega f + \Delta g + \frac{s}{2} \sum_{\alpha=\pm} \frac{i \sigma \alpha s f}{c + i \sigma \alpha s g} = i \omega f + \Delta g + \epsilon s^2 \frac{fg}{c^2 + s^2 g^2} \tag{4} \]

Here, we introduced \( c = \cos(\delta \phi/2) \), \( s = \sin(\delta \phi/2) \) and lumped other parameters into the rate \( \Gamma \). Note that the spin-dependence signaled by \( \sigma \) has dropped out, since \( \hat{g}_\pm \) fulfill the same equations in this case in the absence of an external field.
So we obtain spin-independent Green functions. We can map this exactly onto the Equation \(\xi\) by identifying \(u = ig/f\) with the result

\[
\frac{\omega}{\Delta} = u \left( 1 + i \frac{\epsilon \sin(\phi/2)^2 \sqrt{u^2 - 1}}{\Delta} \frac{\sqrt{u^2 - 1}}{u^2 - c^2} \right)
\]

from which we read the scattering rate of Ref. [32] \(\Gamma = \epsilon \sin(\phi/2)^2\). We have used that \(g = u/\sqrt{u^2 - 1}\) which follows from the normalization condition. Hence, the formulas match exactly and we can identify the Shiba bound state energy \(\varepsilon_B = c = \cos(\delta\phi/2)\), which is exactly expected [33] and the main result here. To illustrate this correspondence we plot two further examples in Fig. 2(c) and (d), where we use two spin-mixing angles of equal weight and magnitude, but opposite sign. In this case, the density of states is spin-degenerate. For weak spin-mixing, an Abrikosov-Gor’kov type broadening of the density of states is observed. The identification of the boundary condition to second order in \(\phi\) with the Abrikosov-Gor’kov pair breaking mechanism has already been noted earlier [19]. The effective pair-breaking rate in this case is given by \(\Gamma = \epsilon \sin(\phi/2)^2\), whereas the effective Zeeman splitting in Fig. 2(a) is given by \(\epsilon \sin(\phi/2)\). Therefore, we chose a larger \(\epsilon\) for Fig. 2(a) to illustrate the pair-breaking effect. Fig. 2(d) shows the case of strong spin-mixing, where the well-known spin-degenerate Shiba bands in the superconducting gap are recovered.

To further explore the consequences of the strongly spin-dependent boundary condition, we study the effect of two interacting Shiba bands. This means we take two types of spin active channels with spin mixing angles \(\phi_1\) and \(\phi_2\). We assume they are described by the effective spin-flip rate \(\epsilon\) and assume the same number of both types of scatters. Some exemplary results are plotted in Fig. 3. In this figure we fix the spin mixing angle of the first band \(\sin \phi_1/2 = 0.85\) and vary the second spin mixing angle. Fig. 3 (a) and (c) show the total density of states for different spin mixing angle with the opposite (a) and the same (c) sign. For the case with \(\sin \phi_2/2 = -0.7\) (black curve), the two Shiba bands are not overlapping in energy and, hence, the total density of states is simply the sum of the two Shiba bands. Note, that the two bands with positive energy have opposite spin polarizations. For the case of opposite spin mixing angles
Figure 3: Effect of two interacting Shiba bands. The weights are taken equal and the spin-mixing parameter of one band is varied. (a) and (c) show the difference between aligned (same sign of $\phi$) and anti-aligned (opposite signs of $\phi$) Shiba impurity bands. The strongly different behaviors can be explained by the spin-resolved densities of states in (b) and (d). Whereas the equal-spin impurity band strongly hybridized in (d), the oppositely polarized bands cross without interaction.

\[
\sin \frac{\phi_2}{2} = -\sin \frac{\phi_1}{2} \quad \text{(green curve)},
\]

the bands are at the same energy and, according to the argument before, the total density of states is unpolarized. For the case of almost similar magnitudes of the spin mixing angles $\sin \frac{\phi_2}{2} = -0.85$, the total density of states has a nontrivial shape with a central peak emerging in a broad background. This behavior can be explained by looking at Fig. 3(b) showing the spin-resolved density of states, which do not interact in the overlap regime, giving ride to the peculiar peaked behavior of the total density of states in this case. In Fig. 3(b) we show the case of two similar spin
mixing angles of similar size and the same sign. Obviously nothing prevents the two equally polarized Shiba bands to interact at the same energy, which results in a simply hybridization in the case of almost equal spin mixing angles (red curve in Fig. 3 (c)). In this case the Shiba bands remain spin-polarized, as is illustrated in the Fig. 3 (d). Finally, we note that the case of equal of the spin mixing angle (green curve in Fig. 3 (c)) differs quantitatively from the case case of opposite signs (green curve in Fig. 3 (a)).

In conclusion, we have show that the strongly spin-dependent scattering at an interface to a magnetic insulator has a similar effect as scattering of spinfull impurities, which lead to the formation of Yu-Shiba-Rusinov states.

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