Spontaneous Spin Polarized Currents in Superconductor-Ferromagnetic Metal Heterostructures

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We study a simple microscopic model for thin, ferromagnetic, metallic layers on semi-infinite bulk superconductor. We find that for certain values of the exchange splitting, on the ferromagnetic side, the ground states of such structures feature spontaneously induced spin polarized currents. Using a mean-field theory, which is selfconsistent with respect to the pairing amplitude $\chi$, spin polarization $\vec{m}$ and the spontaneous current $\vec{j}$, we show that not only there are Andreev bound states in the ferromagnet but when their energies $E_{\alpha}$ are near zero they support spontaneous currents parallel to the ferromagnetic-superconducting interface. Moreover, we demonstrate that the spin-polarization of these currents depends sensitively on the band filling.

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Recently it has become possible to fabricate high-quality interfaces between superconductors (SC) and a metallic Ferromagnets (FM)\[1\]. Evidently the proximity effect in such SC/FM hybrid structures is of scientific interest since it facilitates the study of coexistence between magnetism and superconductivity \[3\]. Furthermore, it may also become technologically important in connection with magnetoelectronics \[3\] and quantum computing \[3\]. In this letter we report on our study of this intriguing phenomenon in a ferromagnetic layers on a bulk superconductor with a particular focus on one of its novel physical features, a spontaneously induced current in the ground state, which is relevant form both points of view.

Clearly, in the present context the ‘proximity effect’ means both the leakage of superconductivity into the non-superconducting, ferromagnetic metal and the spin polarization of the superconductor near the interface. In the analogous case where the normal metal is non-magnetic (NM) this effect has been studied for a long time and is, by now, well understood \[3\]. By contrast, the experimental and theoretical interest in the SC/FM heterostructures and interfaces is more recent and the subject is correspondingly less well developed. Nevertheless, a number of the new phenomena, associated with Cooper pairs in an exchange field, have been identified. For instance, it has been found that, as opposed to the SC/NM case, the pairing amplitude $\chi$ does not decay exponentially to zero on the ferromagnetic side of a SC/FM interface but oscillates, with a slowly decreasing amplitude, as a function of the distance $d$ from the interface \[10,11\]. These oscillations turn out to be manifestations of the effect first studied by Fulde and Ferrel \[10\] and Larkin and Ovchinikov \[11\], often referred to as FFLO, and some of their more striking consequences, such as the oscillation of the superconducting transition temperature $T_c$ as a function of the thickness of the FM layer has been observed experimentally \[13\].

Our work is particularly relevant to the predicted \[13,14\] and observed \[15\] Andreev bound states in clean thin ferromagnetic films sandwiched between two superconductors. Interestingly, these states were found to form part of the ground or equilibrium states and to give rise to so called $\pi$-states of the SC/FM/SC interface. One of the aim of this letter is to argue that a hitherto overlooked salient feature of such FFLO $\pi$-junction is a spontaneous current parallel to the FM/SC interface. We shall also show that the spin polarization of such current depends sensitively on whether the state has, or has not, particle-hole symmetry.

To investigate the occurrence spontaneous currents and their polarization in a SC/FM heterostructure we need a model simple enough to be solved, at least in a mean-field approximation, for the magnetization $\vec{m}$, pairing amplitude $\chi$ and spontaneous current $\vec{j}$ self-consistently. Hence, for the purpose at hand, we have adopted a single orbital, nearest neighbour hopping, negative $U$ Hubbard model for describing the semi-infinite superconductor and continued the same Hamiltonian into the ferromagnetic layer with the $U$ set equal to zero and the site energies $\varepsilon_{i\sigma}$ exchange split. Moreover, we consider the simplest geometry, depicted in Fig.\[3\], where a magnetic field in one direction, the vector potential and a current in another and a spatial modulation in a third orthogonal direction can be realised. Hopefully, while simplify-

![FIG. 1: Schematic view of the superconductor-ferromagnet interface. Directions of the magnetic field (B) as well as vector potential (A) and current (J) are indicated.](image-url)
ing the calculation this effectively 2D system will have much in common with its 3D counterpart such as a layer of ferromagnetic metal deposited on a superconducting substrate \[ \[ \] \] and corresponding sandwich structures \[ \[ \].

In short, our model Hamiltonian is given by

\[
H = \sum_{ij\sigma} [\varepsilon_{ij\sigma} - \mu] \delta_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} \frac{U_i}{2} n_{i\sigma} \hat{n}_{i-\sigma} \tag{1}
\]

where, in the presence of a vector potential \( \vec{A}(\vec{r}) \),

\[
t_{ij} = -ie^{-i\vec{r}_i \cdot \vec{A}(\vec{r})} \delta_{ij}
\]

for nearest neighbour lattice sites at spatial positions \( \vec{R}_i \) and \( \vec{R}_j \), the site energies \( \varepsilon_{i\sigma} \) are 0 on the superconducting side and equal to \( \frac{1}{2} E_{C\bar{\sigma}} \) on the ferromagnetic side, \( \mu \) is the chemical potential, \( U_i \) is \( U_S < 0 \) in the superconductor and zero elsewhere, \( c_{i\sigma}^\dagger \) (\( c_{i\sigma} \)) are the usual electron creation (annihilation) operators and \( \hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \). Note that the above description of the electrons with charges \( e \) includes a coupling to a magnetic field \( \vec{B}(\vec{r}) = \vec{\nabla} \times \vec{A}(\vec{r}) \). Evidently such provision will be necessary for calculating the effects of currents on the electronic states.

In what follows we shall study the above model in the Spin-Polarized-Hartree-Fock-Gorkov (SPHFAG) approximation. We shall work in the Landau gauge where \( \vec{B} = (0, 0, B_z(x)) \) and hence \( \vec{A} = (0, A_y(x), 0) \). Furthermore, we assume that the effective SPHFAG Hamiltonian is periodic in the direction parallel to the interface and therefore we work in \( k \) space in the \( y \) direction but in real space in the \( x \)-direction (see Fig. 1). Labeling the planes in Fig. 1 by integers \( n \) and \( m \) at each \( k_y \) point of the Brillouin zone we shall solve the following SPHFAG Nambu, spin (\( \alpha \)) and layer index (\( n \)) matrix equation:

\[
\sum_{m',\gamma,k_y} H_{nm\gamma}^{\alpha\gamma}(\omega, k_y) G_{m'm}^{\gamma\beta}(\omega, k_y) = \delta_{nm} \delta_{\alpha\beta} \tag{2}
\]

where the only non-zero elements are: \( H_{nm}^{11} \) and \( H_{nm}^{22} = \omega - \frac{1}{2} E_{C\bar{\sigma}} \pm \mu \pm i \cos(k_y + eA(n)) \delta_{nm} \pm i \delta_{n,-1} \) for the upper and lower sign respectively, \( H_{nm}^{33} = H_{nm}^{11} \) and \( H_{nm}^{44} = H_{nm}^{22} \) with \( \sigma \) replaced by \( -\sigma \) in both cases, \( H_{nm}^{12} = H_{nm}^{21} = -H_{nm}^{34} = -H_{nm}^{43} = \Delta_0 \delta_{nm} \) and \( G_{nm}^{\alpha\beta} \) is corresponding retarded Green’s function (\( GF \)).

As usual, selfconsistency is assured by the relation:

\[
\Delta_n = U_n \sum_{k_y} (c_{n\uparrow}(k_y)c_{n\downarrow}(k_y)) = -U_n \sum_{k_y} \int d\omega \frac{1}{\pi} \text{Im} G_{nm}^{12}(\omega, k_y) f(\omega) \tag{3}
\]

where \( f(\omega) \) is the Fermi distribution function. Moreover, the \( FM \) order parameter is given by

\[
m_n = \frac{1}{2}(n_{n\uparrow} - n_{n\downarrow}) = -\frac{1}{2\pi} \sum_{k_y} \int d\omega \text{Im}(G_{nm}^{11}(\omega, k_y) - c_{n\uparrow}(k_y)) f(\omega) \tag{4}
\]

Since our model includes a vector potential the solution of Eq. 2 will imply a current. For spin up electrons, in the \( y \)-direction this can be calculated from the relation:

\[
J_{y\uparrow}(n) = -2\pi \sum_{k_y} \sin(k_y - eA_y(n)) \times \int d\omega \frac{1}{\pi} \text{Im} G_{nm}^{11}(\omega, k_y) f(\omega) \tag{5}
\]

which follows from the continuity equation for the charge.

Finally, the above current will give rise to a vector potential \( A_{\text{env}}(\vec{r}) \) which will have to be used to update \( \vec{A}(\vec{r}) \) in Eq. 2 at the end of each selfconsistency cycle. We calculated this new vector potential by solving numerically Ampere’s law, \( \partial A_y(x)/\partial x = -4\pi J_y(x) \), which for the lattice problem at hand, is

\[
A_y(n + 1) - 2A_y(n) + A_y(n - 1) = -4\pi J_y(n) \tag{6}
\]

We have solved Eqs. 2-5 using an appropriately simplified ‘principal layers method’ \[ \] which we shall describe elsewhere \[ \]. The rest of this letter is a brief summary of our results.

Firstly, since we determined the order parameters, \( \chi_n \) and \( m_n \), on both sides of the interface fully self-consistently, we were able to study both a superconducting and a magnetic proximity effects. Although \( \Delta_n = 0 \) on the ferromagnetic side, due to the fact that \( U = 0 \), the pairing amplitude \( \chi_n = \langle c_{n\uparrow}c_{n\downarrow} \rangle \) does not have to be, and indeed it turns out not to be, zero. Given the well understood effect of the exchange field in a bulk superconductor \[ \], it is not altogether surprising that we find that on entering into the ferromagnet \( \chi_n \) oscillates as a function of the distance from the interface. In fact our numerical results fit the analytic formula \( \chi(x) \sim \sin(x/\xi_F)/(x/\xi_F) \), where \( \xi_F = t/E_{C\bar{\sigma}} \) is the ferromagnetic coherence length, and hence are fully consistent with those of Ref. \[ \]. The rest of this letter is a brief summary of our results.

Of course, the most remarkable feature of the above solution is that the iterations of the \( SPHFAG \) equations frequently converge to a finite value of the current \( J_y(n) \) even though the external vector potential is zero. We have checked that the existence of such spontaneous current lowers the energy of the system. As shown in Fig. 2.
it flows in the positive y direction on the ferromagnetic side, and in negative in the superconductor and sums, reassuringly, to zero over all layers. We have also found numerically, that there is a magnetic flux $\Phi \approx \Phi_0/2$, $\Phi_0$, being the flux quantum, associated with this current distribution.

To shed light on the origin of the above spontaneous current, in Fig. 3 we also show the layer resolved density of states, namely the spectral function $\rho_n(\varepsilon_F) = -\frac{1}{\pi} \sum_k \text{Im}(G_{nn}(\varepsilon_F, k))$, at the Fermi energy $\varepsilon_F$. Clearly, the oscillations of the layer resolved current tracks those of the density of states. Further insight follows if we compare this with the corresponding quantity, denoted by $\rho_\theta(\varepsilon_F)$ and represented by the dot line, in the case where the exchange splitting, $E_{ex}$, is set equal to zero. Since the rise and fall of $\rho_\theta(\varepsilon_F)$ across the ferromagnetic layer can be readily interpreted as the order parameter amplitude of an Andreev bound state, corresponding to the semiclassical path depicted in the inset of the Fig. 3, we can regard $\chi_n$ in Fig. 2 and $\rho_n(\varepsilon_F)$ in Fig. 3 as an indication that a similar bound state is formed in the much more complicated case of finite exchange field. In fact we can identify such FFLO-Andreev bound states as peaks in the full quasiparticle density of states for the ferromagnetic layers. As might be expected these are exchange split and move around as a function of the exchange field $E_{ex}$. Investigating the correlation between such bound states and the current carrying capacity of a solution we find that in the ground state a current flows only when the energy of one of the FFLO-Andreev bound state is near the Fermi energy. Furthermore, in the presence of the current, this state splits, thus lowering the total energy of the system. An example of such zero energy bound state is depicted in the inset of the Fig. 3.

Zero energy Andeev bound states in SC/NM/SC junctions usually lead to a so called $\pi$-states of the two superconductor in which the phases of their order parameters differ by $\pi$. Recently, Chhtchelkatchev et al. [21] suggested that the same is true for a SC/FM/SC junction in the presence of fully developed FFLO phenomena. Interestingly, although the structure we have been studying has only one superconducting region it turns out to display properties analogous to those of such $\pi$-junctions. To see these we studied the order parameter $\chi_{-9}$ at the surface of the ferromagnetic layer opposite to the superconductor. Since $\chi_n$ is negative in superconductor when $\chi_{-9}$ is positive we may describe the system as being in a $\pi$-state. In Fig. 4 we display our results for $\chi_{-9}$ as a function of the dimensionless exchange field $\Theta = 3dE_{ex}/\pi t$ ($d$ is the number of FM layers). Evidently, there are regions of $\Theta$ for which the system can be said to be in $\pi$-state, in close agreement with the analogous results of Chhtchelkatchev et al. [21].

Remarkably, the states with spontaneous currents correspond to regions of the exchange field $\Theta$ where the order parameter $\chi_{-9}$ is near zero. As can be easily read
off from these plots, in these regions the presence or absence of the currents have a dramatic effect on the order parameter. Evidently, the spontaneous current pins the order parameter on the non-superconducting side of the ferromagnetic layer (χ-ex) to zero. This appears to stabilise the zero energy FFLO-Andreev bound state. Given their physical origin one might expect the above spontaneous currents to be spin polarised. This is indeed the case. In fact, we find that the degree of spin polarization is largely determined by the difference in the spin up and spin down densities of state at the Fermi energy: \[ Δρ_n = ρ_n↑(E_F) − ρ_n↓(E_F). \] In the above calculations we have assumed a half filled band, that is to say particle hole symmetry, and hence we have found no difference between the spin up and spin down currents. However, further calculations, away from particle hole symmetry, revealed much larger spin polarizations. An example of this is reported in Fig. 5.

In summary, we have demonstrated that zero energy Andreev bound states in ferromagnetic layers deposited on a superconducting substrate will carry currents in the ground state of such a hybrid structure. Moreover, we found that such states will form only in certain regions of the exchange field \( E_{ex} \) and layer thickness \( d \) phase diagram. In particular, we investigated the cases \( 0 < E_{ex} / t < 3, 0 < d < 20 \). Finally we found that the spin polarization of the current is closely related to the difference in the spin up and spin down density of states at the Fermi level.

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