Origin of Spontaneous Currents in a Superconductor-Ferromagnet Proximity System

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Abstract

We have previously shown that a ferromagnet-superconductor heterostructure may possess a spontaneous current circulation parallel to the interface. This current is caused by Andreev bound states in the thin ferromagnetic layer, and can be fully spin-polarized. Here we investigate the total energy of the system in cases where the current either does or does not flow. We show that the current is a true quantum ground state effect, and examine the effect of the current on the different contributions to the total energy.

Key words: proximity effect, superconductor-ferromagnet interface

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The proximity effect between a superconductor and a ferromagnet has been a subject of great interest in recent years. Unlike the usual proximity effect between a superconductor (S) and a normal metal, a superconductor in contact with a ferromagnet (F) is subject to time reversal symmetry breaking which splits the up and down spin components of the spin-singlet Cooper pairs. In bulk superconducting materials a ferromagnetic exchange splitting leads to the FFLO (or LOFF) state in which the superconducting order parameter oscillates in space[1,2]. In hybrid S-F structures the same physical effect also leads to spatial oscillations[3]. This gives rise to a number of new phenomena, including: Josephson $\pi$-junction behaviour in S-F-S heterostructures[4,5], a giant mutual proximity effect in S-F nanostructures[6], and spin valve[7]

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Fig. 1. The model system we consider. The ferromagnet (FM) consists of $d$ atomic layers ($x = -d, \ldots, 0$), and is in contact with a semi-infinite superconductor ($x = 1, 2, \ldots$). A current, $J$, may flow along $y$, parallel to the surface. This current leads to a magnetic vector potential $A$ in the same direction, and to a $B$-field in the $z$ direction perpendicular to the current, as shown.

and giant magnetoresistive (GMR) effects[8]. In addition to direct proximity effects there are also magnetic interaction effects between the $B$-field of the ferromagnet and the Meissner screening currents of the superconductor. These lead to the pinning of superconducting vortices by magnetic domains in S-F bilayers[9] and by patterned arrays of ferromagnetic nanodots[10]. More complex topological order parameter textures have also been predicted[11]. Lyuksyutov and Pokrovsky have recently reviewed this rapidly expanding literature[12].

We have recently examined the S-F proximity effect in the simple model system shown in Fig. 1[13,14,15]. This represents a bulk superconductor with a thin ferromagnetic layer on the surface. By solving the Bogoliubov de Gennes equations self-consistently for this system we found that the proximity effect leads to an oscillatory superconducting pairing amplitude

$$\chi(r) \equiv \langle c^\dagger_r \sigma, c_r \sigma \rangle \propto \frac{\sin(x/\xi_F)\sqrt{x/\xi_F}}{x/\xi_F} \quad (1)$$

within the ferromagnetic layer. Here $c_{r\sigma}$ is the usual electron annihilation operator at lattice site $r = (x, y)$ and $\xi_F = 2t/E_{ex}$ is the ferromagnetic coherence length with $t$ the hopping and $E_{ex}$ the Stoner exchange splitting within the ferromagnet. This oscillatory component has the same origin as the inhomogenous FFLO superconducting state, essentially a breaking of time reversal symmetry of the Cooper pairs, and is consistent with experiments such as those of Kontos et al.[3]. The damping of the oscillations as a function of distance from the S-F interface is the same as in the usual proximity effect with non-magnetic metals, simply the decay of the Cooper pairs in the non-superconducting material.

We also found a much more surprising feature of the system shown in Fig. 1, namely a spontaneous spin-polarized current, $J$, parallel to the S-F interface[13,14,15]. An unexpected feature of this current is that it switches on or off suddenly as
a function of the number of ferromagnetic layers, \( d \), divided by the coherence length \( \xi_F \). In fact we found the stable self-consistent solution of the Bogoliubov de Gennes equations has a finite current precisely when the dimensionless parameter, \( \Theta = 2.79dE_{ex}/(\pi t) \) is equal to an odd integer, \( n = 1, 3, 5, \ldots \). This surprising condition precisely corresponds to the conditions for the superconducting order parameter at the top ferromagnetic layer \( \chi(-d, 0) \) to be zero. As shown in [15] the top layer order parameter \( \chi(-d, 0) \) oscillates as a function of \( E_{ex} \), changing sign whenever \( \Theta \) is an odd integer. Further analysis showed that this unusual condition for the current carrying solution arises from the spectrum of the Andreev bound states within the ferromagnetic layer. An instability arises whenever a pair of Andreev bound states become degenerate at the Fermi level. The self-consistent solution with the current flow splits the degenerate pair, and leads to a spontaneous parallel current flow, \( J \) along the S-F interface.

In this paper we investigate in more depth this surprising sudden turning on and off of the current carrying solution. We calculate the total energy of the system shown in Fig. 1 both with and without the current flow. This allows us to explain more clearly the physical origin of the current, and to confirm that the current is indeed a true quantum ground state effect. In the next sections we first outline the formalism and computational methodology and for our calculations, before we then present the results.

Our model Hamiltonian is given by the negative \( U \) Hubbard model,

\[
H = \sum_{ij\sigma} [t_{ij} + (\varepsilon_{i\sigma} - \mu) \delta_{ij}] c_{i\sigma}^+ c_{j\sigma} + \sum_{i\sigma} \frac{U_i}{2} \hat{n}_{i\sigma} \hat{n}_{i-\sigma},
\]

where, the nearest neighbour hopping integrals are \( t_{ij} = -te^{-ie \int_{\vec{r}_i}^{\vec{r}_j} \vec{A}(\vec{r}) \cdot d\vec{r}} \) in the presence of a vector potential \( \vec{A}(\vec{r}) \). The site energies \( \varepsilon_{i\sigma} \) are 0 on the superconducting side and equal to \( \frac{1}{2}E_{ex}\sigma \) on the ferromagnetic side, \( \mu \) is the chemical potential, and \( U_i \) is \( U_S < 0 \) in the superconductor and zero elsewhere. Here \( c_{i\sigma}^+, (c_{i\sigma}) \) are the usual electron operators and \( \hat{n}_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} \).

We solve the above model in the Spin-Polarized-Hartree-Fock-Gorkov (SP-HFG) approximation. We work in the Landau gauge where \( \vec{B} = (0, 0, B_z(x)) \) and hence \( \vec{A} = (0, A_y(x), 0) \) (see Fig.1). Furthermore, we assume that the effective \( SPHFG \) 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. As usual, self-consistency is assured by the relation:

\[
\Delta_n = U_n \sum_{k_y} \langle c_{n\downarrow}(k_y) c_{n\uparrow}(k_y) \rangle = -U_n \sum_{k_y} \int d\omega \frac{1}{\pi} \text{Im} G_{nn}^{12}(\omega, k_y) f(\omega)
\]
Fig. 2. The difference in total energy between solutions with and without current flow. The difference is large whenever the parameter $\Theta = 2.79dE_{ex}/(\pi t)$ is an odd integer, and the current flow is stable. For other values of $\Theta$ the energy difference is zero, and no current flow occurs.

where $G^{\alpha\beta}_{nm}(\omega, k_y)$ is the $4 \times 4$ Nambu Green function and $f(\omega)$ the Fermi function.

Since our model includes a vector potential the solution may imply a non-zero current. For spin up electrons, in the $y$-direction this can be calculated from:

$$J_{y\uparrow(\downarrow)}(n) = -2et \sum_{k_y} \sin(k_y - eA_y(n)) \int d\omega \frac{1}{\pi} \text{Im}G_{nn}^{11(33)}(\omega, k_y)f(\omega).$$  \hspace{1cm} (4)

The current will give rise to a vector potential $A(\vec{r})$ which is obtained solving Ampere’s law, $\frac{d^2A_y(x)}{dx^2} = -4\pi J_y(x)$. This full set of equations can be solved self-consistently, using the method described in [15]. The various contributions to the total free energy can also be calculated, and the expressions for the various contributing terms are given in [16].

The coupled set of non-linear equations given above can be solved self-consistently both with and without a finite current flow, $J$. Fig. 2 shows the change in total energy of the system in Fig. 1 between the fully optimized self-consistent solution and the one where the current is constrained to be zero. We used the parameter values: $d = 20$ layers, temperature $T = 0.01$ and $U = -2.345$ in units of the hoping integral $t$. Comparing the total energy of these two cases we can see, in Fig. 2 that the current carrying solution is indeed the one of lower total energy, when the current carrying state is found. These are the series of sharp minima, each one occurring where the dimensionless parameter $\Theta$ (defined above) is an odd integer, and where the pairing order parameter $\chi(\vec{r})$ changes sign on the topmost layer of the ferromagnet.

In between these sharp minima, the energy difference goes to zero, because when $\Theta$ is away from odd integer values the ground state has no spontaneous current flow. One can also see in Fig. 2 that the magnitude of the energy
difference gradually declines as the exchange splitting $E_{ex}$ becomes larger. This is because the oscillatory $\chi(\mathbf{r})$ in the ferromagnet (Eq. 1) becomes more and more heavily damped as the exchange splitting increases. The energy gain associated with the current declines, and for very large $E_{ex}$ the spontaneous current $J$ is suppressed. The modulations in the size of the energy gain shown in Fig. 2 are due to oscillations in the amplitudes of the Andreev states in the density of states at the Fermi energy.

One can analyze these contributions further by examining the various terms contributing to the total energy. In Fig. 3 we show the change in electron kinetic energy $\langle t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma} \rangle$. Clearly this is very similar in magnitude and form to the total energy change of Fig. 2, showing that the spontaneous current is mainly driven by the desire to lower the electron kinetic energy. Other contributions to the total energy change, such as the 'gap' term, $\sum_i |\Delta_i|^2/U_i$, shown on the right in Fig. 3 are not only smaller in magnitude, but can also be either positive or negative. This shows that the spontaneous current flow has only a marginal effect on these contributions to the total energy.

In conclusion we note that these results are consistent with the picture developed in Ref. [15]. The spontaneous current flow is generated to lift a Fermi surface degeneracy between Andreev bound states, and is primarily driven by kinetic energy optimization among the Andreev bound states. The conditions for this current to be observable experimentally are (i) that the ferromagnetic exchange $E_{ex}$ be not too large (i.e. a weak ferromagnet), (ii) the ferromagnetic thin film thickness should be thinner than the electron mean free path, $d < l$ [17], and (iii) the F-S interface transparency must be greater than about $\eta > 0.3$ [17]. In systems satisfying these conditions, the existence of the spontaneous current may be confirmed experimentally by observing the related magnetic flux $\sim 0.0125\Phi_0$ per plaquette, or by STM spectroscopy on the Andreev states near to the Fermi level[15].
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