Andreev Bound States in Ferromagnet - Superconductor Nanostructures *

M. Krawiec *, B. L. György and J. F. Annett

**H. H. Wills Physics Laboratory, University of Bristol,**
**Tyndall Avenue, Bristol BS8 1TL, UK**

**Abstract**

We discuss the properties of a ferromagnet - superconductor heterostructure on the basis of a Hubbard model featuring exchange splitting in the ferromagnet and electron - electron attraction in the superconductor. We have solved the spin - polarized Hartree - Fock - Gorkov equations together with the Maxwell’s equation (Ampere’s law) fully self-consistently. We have found that a Proximity Effect - Fulde - Ferrell - Larkin - Ovchinnikov state is realized in such a heterostructure. It manifests itself in an oscillatory behavior of the pairing amplitude in the ferromagnet and spontaneously generated spin polarized current in the ground state. We argue that it is built up from the Andreev bound states, whose energy can be tuned by the exchange splitting and hence can coincide with the Fermi energy giving rise to a current carrying \( \pi \)-state. We also suggest experiments to verify these predictions.

**Key words:** proximity effect, ferromagnetism, superconductivity

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**1 Introduction**

When a non-magnetic normal metal is in contact with a superconductor it acquires superconducting properties. This effect, known as the proximity effect [1], has extensively been studied for almost 40 years, and is rather well understood in terms of Andreev reflections [2]. On the other hand the proximity

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* e-mail address: m.a.krawiec@bristol.ac.uk
effect between a ferromagnet ($FM$) and a superconductor ($SC$) is less understood. However recent advance in nanofabrication made it possible to produce high quality $FM/SC$ interfaces [3] and hence there is much current interest in the study of the interplay between magnetism and superconductivity in heterostructures involving such surfaces [4]-[9].

It is widely accepted that ferromagnetism is destructive for superconductivity. Thus one expects that the proximity effect in a ferromagnet should be very short ranged. Indeed, it has been predicted [10] that Andreev reflections are suppressed due to the fact that impinging electrons and reflected holes occupy bands with different spin orientations. Surprisingly, some of the experiments seem to be in contradiction with the short range nature of the proximity effect. For instance, it was found [4] that the transition temperature $T_c$ of the $FM/SC$ multilayers oscillates as a function of the $FM$ thickness. This curious behavior has been attributed to the formation of an effective $\pi$-junction [11].

In general a system is in the $\pi$-phase if the $SC$ order parameter changes its sign across the junction. The $\pi$-junction behavior has been extensively studied in connection with the high-$T_c$ superconductors [12], where $SC$ order parameter changes its sign under $\pi/2$ rotation. This has tremendous consequences as it leads to the zero energy Andreev states [13], zero bias conductance peaks, paramagnetic Meissner effect and spontaneously generated currents.

Some other experiments show oscillatory behavior of the $T_c$, even though a $\pi$-junction cannot be realized in the geometry investigated. The example is a $FM/SC/FM$ trilayer [6], where only one $SC$ layer is present. Recently oscillations of the density of states with $FM$ thickness in a $FM/SC$ bilayer has been also observed [7]. Evidently a conventional $\pi$-junction is also impossible in this case. Interestingly, such unusual behavior can be explained in terms of a Fulde - Ferrell - Larkin - Ovchinnikov ($FFLO$) - like state [14], forming in the proximity conditions.

Usually, when the exchange field is increased, one would expect that either the field is too weak to break Cooper pairs or it leads through first order phase transition to the normal state. However as it was noted in [14], for certain values of the exchange field a new superconducting state can be realized. This $FFLO$ state features a spatially dependent order parameter and the current flow in the ground state. The total current consists of two contributions: one, which is due to the normal unpaired electrons and the other one, which is a supercurrent. These two parts cancel each other, so the Bloch theorem: no current in the ground state, is satisfied.

Similarly in the $FM/SC$ heterostructures: the oscillations of the pairing amplitude have been predicted [15]-[18] as well as spontaneously generated current in the ground state [19]. These features give a strong evidence that the
**FFLO state** is really realized in FM/SC nanostructures.

In the present paper we attempt to provide further insights into the physics of FFLO state in FM/SC heterostructures. In particular we investigate the properties of the Andreev bound states, pairing amplitude and the spontaneous current when the temperature is varied. We suggest that temperature measurements of various experimentally accessible quantities can contribute much to the understanding of the superconductivity in FM/SC bilayers. The paper is organized as follows: In the section 2 we introduce a simple model which can handle the main properties of FM/SC systems. Some technical details concerning numerical implementation can be found in a subsequent paper [19]. In sec. 3 the nature of the Andreev bound states is discussed. We also show calculated temperature dependences of various quantities characterizing our system. In particular the density of states, which can be measured experimentally, can unambiguously confirm the current flowing in the ground state. Finally, the conclusions are given in sec. 4.

### 2 The model and the formal structure of the theory

To study the properties of FM/SC system we have adopted the 2D Hubbard model featuring the exchange splitting in the ferromagnet and an electron - electron attraction in superconductor. The Hamiltonian is:

\[
H = \sum_{ij,\sigma} \left[ t_{ij} + \left( \frac{1}{2} E_{ex} \sigma - \mu \right) \delta_{ij} \right] c_{i\sigma}^+ c_{j\sigma} + \frac{1}{2} \sum_{i\sigma} U_i n_{i\sigma} n_{i-\sigma}
\]  

(1)

where in the presence of a vector potential \( \vec{A}(\vec{r}) \), the hopping integral is given by \( t_{ij} = -ie \int_{\vec{r}_i}^{\vec{r}_j} \vec{A}(\vec{r}) \cdot d\vec{r} \) for nearest neighbor lattice sites, whose positions are \( \vec{r}_i \) and \( \vec{r}_j \), and zero otherwise. The exchange splitting \( E_{ex} \) is only non-zero on the FM side, unlike as \( U_i \) (electron - electron attraction) being non-zero only in SC. \( \mu \) is the chemical potential, \( c_{i\sigma}^+ \) (\( c_{i\sigma} \)) are the usual electron creation (annihilation) operators and \( \hat{n}_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} \).

In the following we shall work within Spin - Polarized - Hartree - Fock - Gorkov (SPHF\(G \)) approximation [19] assuming periodicity in the direction parallel to the interface while working in a real space in the direction perpendicular. Labelling the layers by integer \( n \) and \( m \) at each \( k_y \) point of the Brillouin zone we shall solve the following S\(PHFG \) equation:

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

(2)
where the only non-zero elements are: $H_{11}^{nm}$ and $H_{22}^{nm} = (\omega - \frac{1}{2} \sigma E_{ex} \pm \mu \pm t \cos(k_y \mp eA(n))) \delta_{nm} \pm \delta_{n,n+1}$ for the upper and lower sign respectively, $H_{33}^{nm} = H_{11}^{nm}$ and $H_{44}^{nm} = H_{22}^{nm}$ with $\sigma$ replaced by $-\sigma$ and $H_{12}^{nm} = H_{21}^{nm} = -H_{34}^{nm} = -H_{43}^{nm} = \Delta_n \delta_{nm}$ and $G_{nm}^{\alpha\beta}$ is corresponding Green’s function (GF).

As usual, the self-consistency is assured by the relations determining the $FM$ order parameters, current $(J_{y\uparrow(\downarrow)}(n))$ and the vector potential $(A_y(n))$ respectively:

$$m_n = n_{\uparrow} - n_{\downarrow} = \frac{2}{\beta} \sum_{k_y} \sum_{\nu=0}^{2N-1} \text{Re} \left\{ (G_{nn}^{11}(\omega_{\nu}, k_y) - G_{nn}^{11}(\omega_{\nu}, k_y)) e^{(2\nu+1)\pi i / 2N} \right\}$$

$$\Delta_n = U_n \sum_{k_y} \langle c_{n\downarrow}(k_y)c_{n\uparrow}(k_y) \rangle = \frac{2U_n}{\beta} \sum_{k_y} \sum_{\nu=0}^{2N-1} \text{Re} \left\{ G_{nn}^{12}(\omega_{\nu}, k_y) e^{(2\nu+1)\pi i / 2N} \right\}$$

$$J_{y\uparrow(\downarrow)}(n) = \frac{4et}{\beta} \sum_{k_y} \sin(k_y - eA_y(n)) \sum_{\nu=0}^{2N-1} \text{Re} \left\{ G_{nn}^{11(33)}(\omega_{\nu}, k_y) e^{(2\nu+1)\pi i / 2N} \right\}$$

$$A_y(n + 1) - 2A_y(n) + A_y(n - 1) = -4\pi J_y(n) \quad (6)$$

The details of the calculations can be found in [19].

### 3 Results and discussion

Since we have determined the $FM$ (3) and the $SC$ (4) order parameters on both sides of the interface fully self-consistently, we were able to study both $FM$ and $SC$ proximity effects. The $FM$ order parameter (spin polarization) shows the usual Meissner-like behavior in the $SC$ [19], while the $SC$ pairing amplitude oscillates as we increase the thickness of the $FM$ slab [16]-[18]. Similar oscillations are found if we fix the thickness of the $FM$ sample and change the exchange splitting [19]. So this is the first confirmation of the FFLO state in $FM/SC$ heterostructures [16,7].

The interesting physics of such proximity structures is the formation of the Andreev bound states [20]. They are ‘particle in a box’ like states due to the finite thickness of the $FM$ and have been discussed extensively [17,19]. For a normal metal in contact with superconductor these states are symmetrically
located with the respect to the Fermi energy $\varepsilon_F$. When the normal metal is replaced by ferromagnet the position of these states is shifted due to the exchange splitting in $FM$ \[21,17,19\]. This gives a possibility to shift such state to the zero energy ($\varepsilon_F$). Of course we should talk about Andreev bands rather than single states because in the 2D system we are studying, there are the Andreev reflections for different angles with respect to the normal to the interface. In such a situation when the pairing amplitude at the end of the $FM$ slab ($FM/vacuum$ interface) is equal to zero, spontaneous current is generated \[19\]. The current flowing in the system produces a magnetic field, which splits this zero energy state thereby lowering the total energy of the system. If we follow the position of one particular state, forming an Andreev band, as the exchange splitting is increased, there is an additional (Doppler) shift when the current flows. The situation is schematically shown in the Fig. 1. In 2 or 3D geometry the whole Andreev band is split. The energy of such Doppler splitting is determined by the vector potential and in our model is given by $\delta \approx 2e\tau A_y$, where the layer averaged vector potential is given by $A_y = \sum_{n \in FM} A_y(n)/N_F$ for $N_F$ layers.

The splitting of the Andreev bands due to the current flowing can be seen if we plot the surface ($FM/vacuum$) density of states at the Fermi energy ($\rho_{tot}(\varepsilon_F)$). This quantity can be directly measured experimentally using planar tunneling spectroscopy \[7\]. The example of $\rho_{tot}(\varepsilon_F)$ is shown in the Fig. 2. There is a dramatic difference between solution with or without the current (in the later case the spontaneous current is constrained to be zero). In calculations it is readily ascertained but experimentally it would be very difficult to judge if there is a current or not. However a plot of the temperature dependence of the $\rho_{tot}(\varepsilon_F)$ for fixed thickness clearly delineates this difference. At the thicknesses of $FM$ for which the current flows there is a huge drop in the $\rho_{tot}(\varepsilon_F)$ at characteristic temperature $T^* \approx (\xi_S/\lambda)T_c$, where $\xi_S$ and $\lambda$ are coherence length and penetration depth respectively. $T^*$ simply indicates the temperature at which magnetic instability, which leads to the generation of the current, takes the place. Such behavior is depicted in the Fig. 3 and should be observable experimentally. If there is no current the $DoS$ is due to the Andreev band and is almost constant (we are well below $T_c$), and as soon as the current starts to flow the Andreev band splits so we observe a drop in $\rho_{tot}(\varepsilon_F)$. The important point is that $T^*$ and $T_c$ are different temperatures.

As we already mentioned, the spontaneous current generates the magnetic field, which can also be measured experimentally by $SQUID$ techniques. Such spontaneous magnetic flux per unit area in the $y$ direction, parallel to the interface, is defined by $\Phi = \sum_0^\Phi(n) = \sum_0^\Phi(A_y(n+1) - A_y(n))$ and is shown in the Fig. 4 as a function of the thickness of the $FM$ sample. We see that $\Phi$ is larger when $FM$ thickness is smaller and is of order of $10^{-2} - 10^{-1}$ $\Phi_0$, where $\Phi_0 = h/2e$ is the flux quantum. Moreover it seems to show an exponential decay with increasing of the number of $FM$ layers. Similarly, in this case
temperature measurement can provide information on the existence of the spontaneous current. Fig. 5 shows spontaneous magnetic flux for a number of thicknesses of the $FM$ slab. It is worthwhile to note that the behavior of $\Phi$ recalls the temperature dependence of the $SC$ order parameter in the $BCS$ theory.

Before closing the present discussion the following remark concerning the ferromagnet itself is in order. In general we should take into account the effect of the magnetic field coming from the localized moments of ferromagnet. These produce magnetic flux as well as surface currents. This effect could be important when the magnetization is perpendicular to the interface, as in our case. However if we deal with the weak ferromagnet or the sample has short lattice constant, the magnetic flux generated by local moments is much smaller than spontaneous one, and we can neglect this effect. In the present calculations we have taken the exchange splitting $E_{ex} = \Delta_S/2$, so this effect is of minor importance.

4 Conclusions

In conclusion we have studied properties of the ferromagnet - superconductor bilayer. We have shown that such a structure supports Andreev bound states forming Andreev bands, the position of which can be tuned by thickness of the $FM$ sample. When a band crosses the Fermi energy, spontaneous current and magnetic flux is generated. We have found that the state with the current flowing can be experimentally detected measuring the temperature dependence of the density of states or the magnetic flux. We have argued that such current carrying state is a realization of the $FFLO$ state in $FM/SC$ proximity system.

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Fig. 1. Additional (Doppler) splitting of the Andreev bound state due to the current flowing in the $FM/SC$ heterostructure.
Fig. 2. The surface ($FM$/vacuum) density of states at the Fermi energy vs. number of the $FM$ layers. The squares (circles) correspond to the solution without (with) the current.
Fig. 3. The temperature dependence of the surface ($FM/vacuum$) density of states at the Fermi energy for various thicknesses of the $FM$ slab in the figure. The solid (dashed) line corresponds to the solution without (with) the current.
Fig. 4. The total magnetic flux per unit area in the $y$ direction vs. number of the $FM$ layers for $E_{ex}/\Delta_S = 0.5$. $\Phi_0 = h/2e$ is the flux quantum and $a$ is the lattice constant.
Fig. 5. The temperature dependence of the total magnetic flux for thickness of the $FM$ slab $L/\xi_S = 2.6$ (solid), 6 (dashed) and 15 (dotted curve).