Proximity Effects near the Interface between \(d\)-wave Superconductors and Ferro/Antiferromagnets

Kazuhiro KUBOKI

Department of Physics, Kobe University, Kobe 657-8501, Japan

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We study the proximity effects near the interface between a \(d\)-wave superconductor (S) and a ferromagnet (F) or an antiferromagnet (AF). The S-side (F and AF-side) is described by the attractive (repulsive) Hubbard model, and the Bogoliubov de Gennes equation derived within the Hartree-Fock approximation is solved numerically. The superconducting order parameter and the magnetization \((m)\) can coexist near the interface, and the spatial variation of \(m\) induces the spin-triplet \(p\)-wave component in both F and AF cases. The local density of states is also calculated and discussed.

KEYWORDS: unconventional superconductivity, proximity effect, Bogoliubov de Gennes equation, local density of states, \(SO(5)\) theory

Recently the proximity effect of unconventional superconductors has been a subject of intensive study. This is because the interface properties of these superconductors can be quite different from those of conventional (\(s\)-wave) ones due to the nontrivial angular structure of pair wave functions, so that their study is of particular interest. Now many unconventional superconductors are known to exist, and the most famous examples are the high-\(T_c\) cuprates in which the \(d_{x^2-y^2}\)-wave superconducting (SC) state is realized.

In this letter we study the proximity effect between a \(d\)-wave superconductor (S) and a ferromagnet (F) or an antiferromagnet (AF). We examine the possible coexistence of magnetism and superconductivity near the interface. In \(s\)-wave superconductors the coexistence is unlikely or limited because of the full gap in the excitation spectrum, while in the \(d\)-wave case it is not. We will show that the coupling of SC order parameters (OPs) with the magnetization induces a spin-triplet \(p\)-wave component. We also calculate the local density of states (LDOS) to show how the electronic structure changes across the interface.

The system we consider is a two-dimensional \(d\)-wave superconductor (S)/magnet (M) bilayer. The direction perpendicular (parallel) to the interface is denoted as \(x (y)\), and we assume that the system is uniform along the \(y\)-direction except the two-sublattice spin structure in the AF case. We treat the Hubbard model on a square lattice within the Hartree-Fock (HF) approximation to describe the magnetism and superconductivity at zero temperature \((T = 0)\). The crystal \(a\)-axis is taken to be parallel to the \(x\)-direction, i.e., we consider only the [100] interface. The Hamiltonian for the two layers is given by

\[
H_L = -t_L \sum_{\langle i,j \rangle > \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) + \sum_i U_L n_{i\uparrow} n_{i\downarrow} + \sum_{\langle i,j \rangle} V_L [n_{i\uparrow} n_{j\downarrow} + n_{j\uparrow} n_{i\downarrow}], \quad (L = M, S)
\]

where \((i,j)\) and \(\sigma\) denote the nearest-neighbor pairs and the spin index, respectively. Parameters \(t_L\), \(U_L\), and \(V_L\) are the transfer integral, the on-site interaction and the nearest-neighbor interaction, respectively, for the \(L = M, S\) side. The transmission of electrons at the interface is described by the following tight-binding Hamiltonian:

\[
H_T = -t_T \sum_{\langle l,m \rangle > \sigma} \langle c_{l,\sigma}^\dagger c_{m, \sigma} + h.c. \rangle (2)
\]

where \(l (m)\) denotes the surface sites of \(M (S)\) layer, and then the total Hamiltonian of the system is \(H = H_M + H_S + H_T - \mu \sum \langle l \rangle c_{l,\sigma}^\dagger c_{l,\sigma} \) with \(\mu\) being the chemical potential. We have examined the various values of \(t_T / t_M (S)\). The results are qualitatively similar, and the effect of proximity is reduced for smaller \(t_T\) as expected. Thus the discussion is restricted to the case of \(t_T = t_M = t_S \equiv t\) throughout this letter.

The interaction terms are decoupled within the HF approximation

\[
U n_{i\uparrow} n_{i\downarrow} \rightarrow U \langle n_{i\uparrow} \rangle n_{i\downarrow} + U \langle n_{i\downarrow} \rangle n_{i\uparrow} - U \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle,
\]

\[
V n_{i\uparrow} n_{j\downarrow} \rightarrow V \Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + V \Delta_{ij} c_{i\downarrow} c_{j\uparrow} - V |\Delta_{ij}|^2
\]

with \(\Delta_{ij} = \langle c_{i\uparrow} c_{j\downarrow} \rangle\), and \(\Delta_{ij}\) and magnetization \(m_i = \langle n_{i\uparrow} - n_{i\downarrow} \rangle / 2\) are the OPs to be determined self-consistently. Along the \(y\)-direction we introduce two-sublattices \(A\) and \(B\), and carry out the Fourier transformation: \(c_{i\sigma}^\alpha = \sqrt{2/N_y} \sum k e_{x_i,\sigma}^\alpha (k) e^{i k y_i}\) \((\alpha = A, B)\), where \(N_y\) \((N_x)\) is the number of sites along the \(y (x)\) direction. Now we define \(\Delta_{ij} = \langle c_{i\uparrow}^A c_{j\downarrow}^B \rangle (\alpha = A, B)\), \(\Delta_{ij}^{(1)} (x_i) = \langle c_{i\uparrow}^A c_{i+\gamma\downarrow}^B \rangle\), and \(\Delta_{ij}^{(2)} (x_i) = \langle c_{i\uparrow}^B c_{i+\gamma\uparrow}^A \rangle\). Then the mean-field Hamiltonian is written as (hereafter \(x_i\) is abbreviated as \(i\))

\[
H_{MFA} = \sum_k \sum_i \sum_j \Psi_i^k(k) \hat{H}_{ij}(k) \Psi_j^k(k)
\]
where
\[
\tilde{h}_{ij} = \begin{bmatrix}
W^A_{ij}(k) & F^A_{ij}(k) & \tilde{W}_{ij}(k) & F_{ij}(k) \\
F^A_{ij}(k)^* & -W^A_{ij}(k) & F^*_{ij}(k) & -\tilde{W}_{ij}(k) \\
\tilde{W}_{ij}(k) & F_{ij}(k) & W^B_{ij}(k) & F^B_{ij}(k) \\
F_{ij}(k) & -\tilde{W}_{ij}(k) & F^B_{ij}(k) & -W^B_{ij}(k)
\end{bmatrix}
\]
\tag{5}
\]
and
\[
\Psi_i(k) \equiv [c_i^a(k)^t, c_i^d(-k)^t, c_i^B(k)^t, c_i^B(-k)^t].
\tag{6}
\]
with
\[
W_{ij}(k) = -t(\delta_{ij,i+1} + \delta_{ij,-1}) + (U|n_i^a - \mu|)\delta_{ij},
\]
\[
F^a_{ij}(k) = -V\Delta^a_j(\delta_{i,i+1} + \delta_{i,i-1}),
\]
\[
\tilde{F}_{ij}(k) = -\frac{V}{2}[e^{ik}\Delta^y_j(i) - e^{-ik}\Delta^y_j(i)]\delta_{ij}.
\tag{7}
\]

We diagonalize the mean-field Hamiltonian by solving the following Bogoliubov de Gennes (BdG) equation:
\[
\sum_j \tilde{h}_{ij}(k)u_{jn}(k) = E_n(k)u_{jn}(k),
\tag{8}
\]
where \(E_n(k)\) and \(u_{jn}(k)\) are the energy eigenvalue and the corresponding eigenfunction, respectively, for each \(k\). The unitary transformation \(\Psi_i(k) = \sum_n u_{jn}(k)\Gamma_n(k)\) diagonalizes the matrix \(\mathcal{H}_{MF}\), and conversely the OPs \(\Delta_ij\) and \(m_i\) can be written in terms of \(E_n(k)\) and \(u_{jn}(k)\). These constitute the self-consistency equations which will be solved numerically in the following.

In a uniform (bulk) case, the ground-state phase diagram of the repulsive Hubbard model \((U > 0)\) within the HF approximation was examined by Hirsch. There the ferro-, antiferro- and paramagnetic states are obtained depending on the value of \(U/t\) and the electron density. For an attractive case \((V < 0)\), the ground state is a spin-singlet SC state. Depending on the electron density a \(d_{x^2-y^2}\) \((\Delta_d)\) or an extended \(s\)-wave \((\Delta_s)\)-wave SC state is stabilized, and the former is favored near half-filling. \(\Delta_d\) \((\Delta_s)\) can be constructed as a linear combination of \(\Delta_i\)’s in such a way that it changes its sign (is invariant) under \(90^\circ\) rotation in the basal plane.

Now, let us study the M/S bilayer system. We impose the open (periodic) boundary condition for the \(x\) \((y)\) direction, and the typical system size treated is \(N_x \times N_y = 40 \times 40\) to \(60 \times 80\) sites. We use \(t\) as a unit of energy \((i.e., t = 1)\). First we choose \(U_M > 0\), \(V_M = 0\), \(U_S = 0\) and \(V_S < 0\) so that the ferromagnetic and \(d\)-wave superconducting states are stabilized in M and S layers, respectively \((F/S)\) system. In Fig.1 the spatial variations of OPs are shown. It is seen that the magnetization \((m)\) and the SCOP \((\Delta)\) coexist near the interface, and the \(p_x\)-wave component \((\Delta_{px})\) as well as \(\Delta_s\) appears. In general, the OP component different from that in the bulk can be induced due to the scattering of Cooper pairs at an interface (or a surface faced to vacuum). The important point here is that we get the \(p_x\)-wave state which is a spin-triplet (even parity) SC state. This state has pairing OP on the bonds along the \(x\)-direction. The spatial variations of OPs in the AF/S bilayer system are shown in Fig.2. In this case the spin-triplet \(p_y\)-wave component \((\Delta_{py})\) also appears. We will neglect the small \(\Delta_s\) in the following discussions.

The penetration of \(m\) into the S side causes the imbalance of the densities of spin-up and spin-down electrons. Thus electron pairs cannot be formed in singlet channels only, and then the spin-triplet component appears. It is seen that the M side is essentially unaffected by the proximity effect. This is because the Curie (or Néel) temperature is higher than \(T_c\) of superconductivity so that the typical lengths for the decay of the induced OPs are shorter in the M side. Then in the following we will mainly focus on the S side.

We analyze the above results more precisely using the Ginzburg-Landau (GL) theory. \(\text{(The GL theory is not quantitatively valid except near } T_c, \text{ but it can give qualitatively correct results.)} \) The GL free energy in the S layer (in the continuum representation) can be written as
\[
\mathcal{F}_S = \int d^2r \left[ \sum_{j=d,s,p_x,p_y} |\alpha_j|\Delta_j|^2 + K_j|\partial\Delta_j|^2 \right]
\]
\[
+ K_{dp}\left( (\partial_x\Delta_d)(\partial_x\Delta_s)^* - (\partial_y\Delta_d)(\partial_y\Delta_s)^* + c.c. \right)
\]
\[
+ K_{dp}\left( (\partial_x\Delta_p)(\partial_y\Delta_{p_x})^* + (\partial_y\Delta_p)(\partial_x\Delta_{p_y})^* + c.c. \right)
\]
\[
+ K_{dp}\left( (\partial_x\Delta_{p_x})(\partial_y\Delta_{p_y})^* + (\partial_y\Delta_{p_y})(\partial_x\Delta_{p_x})^* + c.c. \right)
\]
\tag{9}
\]
This \(\mathcal{F}_S\) is invariant under all symmetry operations for the square lattice and we have dropped higher order terms. All coefficients in \(\mathcal{F}_S\) are positive definite except \(\alpha_j\) which are given at a temperature \(T\) as, \(\alpha_j = V_S[1 - (V_S/N)\sum_k w_k^2(k)\tan(\xi_k/2T)]/2\xi_k\) for \(j = d, s\) and \(\alpha_j = (V_S/2)[1 - (V_S/N)\sum_k w_k^2(k)\tan(\xi_k/2T)]/\xi_k\) for \(j = p_x, p_y\). Here \(N = N_xN_y, \xi_k = 2t(\cos k_x + \cos k_y) - \mu, w(k) = \cos k_x - \cos k_y, w_p(k) = \cos k_x + \cos k_y, w_{px,y} = \sin k_x(y)\). In the bulk superconductor, the SCOP with the highest \(T_c\) occurs \((T_c\) is given by \(\alpha(T_c) = 0)\) and other components are usually suppressed due to the higher order repulsive coupling to the bulk OP (not shown in \(\mathcal{F}_S\)). Near half-filling \(w_{px,y}(k^2)\) is large (small) on the Fermi surface, and \(\Delta_d\) becomes negative first. This is the reason we obtain the \(d\)-wave state near half-filling. (On the contrary, an extended \(s\)-wave state is favored away from half-filling.)

In the M/S bilayer system, several OPs can coexist and they are not spatially uniform. In the F/S case, \(\partial_x m = 0, \partial_y m = 0\) and \(\Delta_d \neq 0\), so that \(\Delta_{px}\) is induced but \(\Delta_{py}\) is not. On the contrary, in the AF/S system, finite \(\partial_y m\) induces \(\Delta_{py}\) also. The opposite sign of \(\Delta_{px}^*\) and \(\Delta_{px}\), and their oscillating behavior in AF/S system can also be understood as being due to the staggered nature of \(m\). The phases of the induced OPs relative to the bulk one \((\Delta_d)\) are either \(0\) or \(\pi\), since they are determined by the bilinear coupling terms in \(\mathcal{F}_S\). Namely, the state has the \((d_{x^2-y^2} \pm p_x)\)-symmetry near the interface of the F/S system, and \((d_{x^2-y^2} \pm p_x \pm p_y)\)-symmetry in the AF/S case.

It has been proposed that antiferromagnetism and \(d\)-wave superconductivity can be treated in a unified way using \(SO(5)\) symmetry. The present result seems consistent with this theory, since \(m\) penetrates deeper into the S side in the AF/S case than in the F/S case. On the contrary \(\Delta_{px}\) decays faster in the former. The
reason for this is the following. The F/S system studied here is closer to half-filling compared with AF/S system. Then, \( \alpha_{px} \) in \( F_S \) can be closer to zero (though still positive) in the F/S case because the factor \( w_{px}^2 \) is larger on the Fermi surface. The coherence length, which determines the decay of \( \Delta_j \), is given by \( \xi_j = \sqrt{K_j/\alpha_j} \), and then the decay is slower in the F/S case. \( (K_j \) is not so sensitive to the electron density.)

Recently, Honerkamp et al.\(^1\) studied the surface states of \( d \)-wave superconductors. They found that near the \([110]\) surface (faced to vacuum) the staggered magnetization can appear spontaneously, and that the \( p \)-wave as well as the extended \( s \)-wave component can occur. Their state breaks time-reversal symmetry spontaneously and a surface current is generated. The reason the \( p \)-wave OP is obtained in the present case is, however, different from theirs. We consider a \([100]\) surface and if it is faced to vacuum, the magnetization cannot be spontaneously generated, hence no \( \Delta_p \) is obtained. In order to have a finite \( \Delta_p \), for the case of a \([100]\) surface, the proximity effects from the magnets are necessary. Honerkamp et al. found the bound states near the Fermi level, which are different for the spin-up and spin-down components because of local antiferromagnetism. If the \([110]\)-oriented M/S bilayer is treated, the split bound states would also be expected.

Next, we show the results of the local density of states (LDOS). The LDOS at site \( i \in A \) is given by

\[
N^A_\uparrow(i, \omega) = \frac{2}{N_y} \sum_k \sum_n \left| u_{A,i-3,n}(k) \right|^2 \delta(\omega - E_n(k))
\]

\[
N^A_\downarrow(i, \omega) = \frac{2}{N_y} \sum_k \sum_n \left| u_{A,i-2,n}(k) \right|^2 \delta(\omega + E_n(k))
\]

(10) \((\uparrow, \downarrow\) being the spin indices) and \( N^B_\uparrow(i, \omega) \) \( (N^B_\downarrow(i, \omega)) \) is obtained by replacing \((4i - 3) \ (4i - 2) \) in the above equation with \((4i - 1), \ (4i) \). For the F/S case \( N^A = N^B = N^B_\sigma = N^B_{\sigma} \) \((\sigma = \uparrow, \downarrow)\). In figures 3 and 4 (5 and 6), the results for the F/S (AF/S) system are shown. Deep inside the F (AF) layer, the LDOS for spin-up and the spin-down components is split as a result of magnetic orders (Fig.3 (Fig.5)). The spin-up and spin-down components gradually merge as the interface is crossed, and a \( V \)-shaped DOS which is typical of a \( d \)-wave superconductor is formed. These changes of the LDOS as a function of the position appear smooth.

In summary we studied the proximity effects near the interface between \( d \)-wave superconductors and ferro/antiferromagnets. We found the coexistence of the magnetic order and the superconductivity, which leads to the \( (d_{x^2-y^2} \pm p_x) \)-wave and \( (d_{x^2-y^2} \pm p_x \pm p_y) \)-wave surface states in the F/S and AF/S systems, respectively. The LDOS changes smoothly from magnetic to SC layers. In this letter we did not take into account the effect of a vector potential that couples to the magnetization in the ferromagnetic state. This coupling may lead to more drastic effects, and is most suitably treated by field theoretical methods. Such an effective theory can be constructed based on the knowledge of the present solutions of BdG equations. This problem will be examined separately in the near future.

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**Fig. 1** Spatial variations of OPs for a F/S bilayer. Here \( U_M = 10, U_S = 0, V_M = 0, V_S = -2 \) and \( \mu = -0.1 \). Note that all OPs are non-dimensional.

**Fig. 2** Spatial variations of OPs for an AF/S bilayer. Here \( U_M = 4, U_S = 0, V_M = 0, V_S = -2, \) and \( \mu = 1 \). (a) \( \Delta_d, \Delta_s, \) and \( m_{A(B)} \), (b) \( \Delta_p^{A(B)}, \Delta_p^{py}, \Delta_d \). Indices A and B denote the sublattice.

**Fig. 3** LDOS for a F/S bilayer. The parameters are the same as in Fig.1 and the finite width \( \Gamma = 0.08 \) is...
introduced to each state. (a) $x = -9a$ with $\sigma = \uparrow$; (b) $x = -9a$ with $\sigma = \downarrow$, (c) $x = 21a$ ($\sigma = \uparrow$ and $\downarrow$ are almost degenerate). Here, $a$ is the lattice constant and $x = 0$ corresponds to the surface site of the M layer.

**Fig. 4** LDOS for a F/S bilayer. The parameters are the same as in Fig. 3 except $x = a$. (a) $\sigma = \uparrow$, (b) $\sigma = \downarrow$.

**Fig. 5** LDOS for an AF/S bilayer. The parameters are the same as in Fig. 2 and the finite width $\Gamma = 0.08$ is introduced. (a) $x = -9a$ with $\sigma = \uparrow$; (b) $x = -9a$ with $\sigma = \downarrow$, (c) $x = 11a$ ($\sigma = \uparrow$ and $\downarrow$ are almost degenerate).

**Fig. 6** LDOS for an AF/S bilayer. The parameters are the same as in Fig. 5 except $x = a$. (a) $\sigma = \uparrow$, (b) $\sigma = \downarrow$. 
Fig 2b
Fig. 3
Fig. 4
Fig. 6